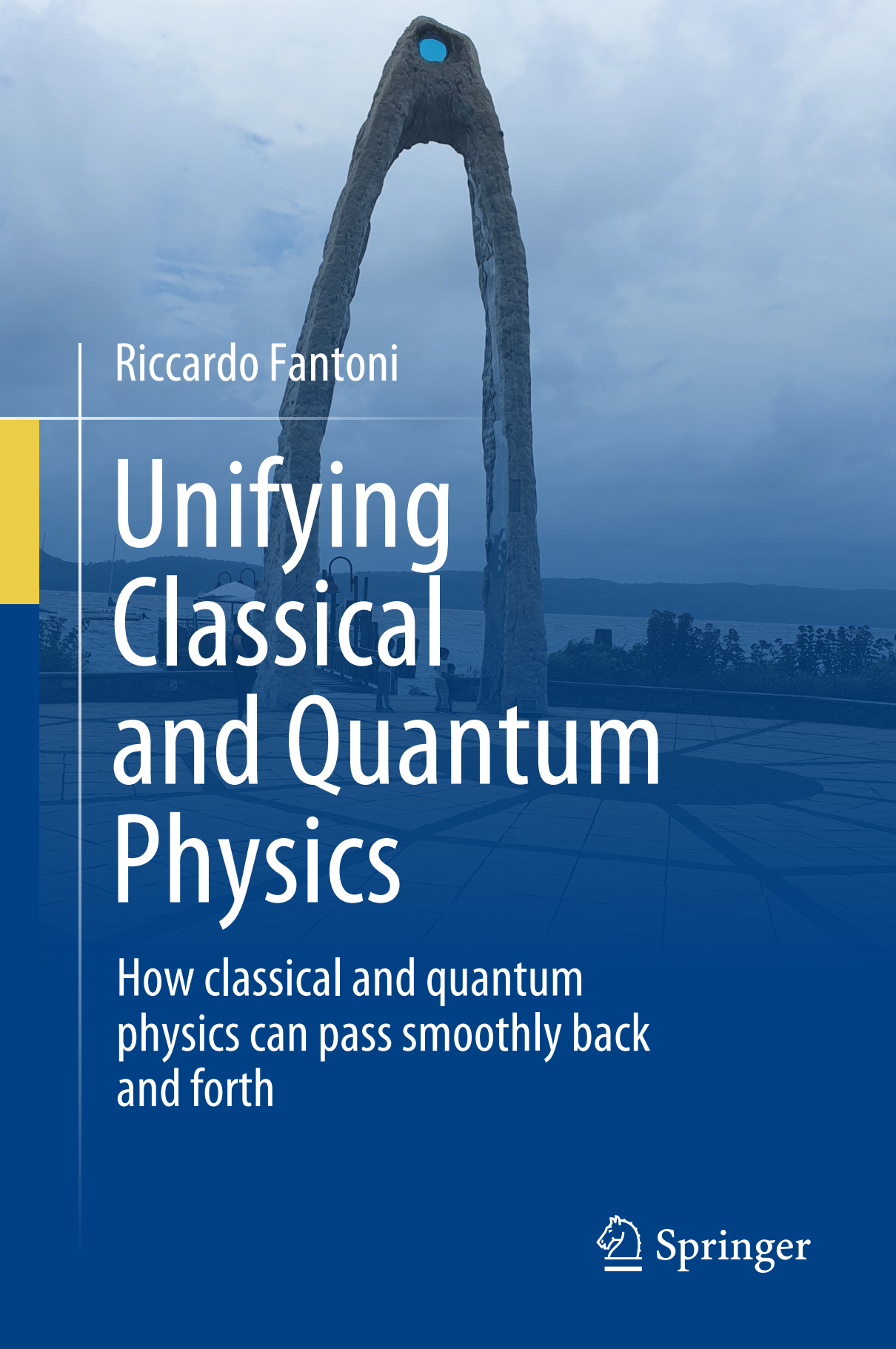




Riccardo Fantoni

Unifying Classical and Quantum Physics

How classical and quantum
physics can pass smoothly back
and forth

Unifying Classical and Quantum Physics



Terzo Paradiso (2019)

Michelangelo Pistoletto

Newspaper on wooden structure, cm 500 × 250 × 35. Matera, University campus, First pavilion.

Realization: Raffaele Pentasuglia e Massimo Caciello

Riccardo Fantoni

Unifying Classical and Quantum Physics

How classical and quantum physics can pass
smoothly back and forth

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*Tra un fiore colto e l'altro donato
l'inesprimibile nulla
Giuseppe Ungaretti
from the poem "Eterno"*

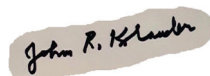
To my daughter Alice

Foreword

Canonical quantization has served well, but it cannot do many problems of interest. The example of the particle in a box fails its effort to deal with quantization using the standard canonical quantization. There is now a new quantization procedure, called affine quantization, which has been constructed and found to be a wonderful tool in solving problems not suitable for canonical quantization. In this case, is perfectly designed to handle the particle in the box. Not only quantum mechanics, can be treated perfectly, affine quantization is also the proper tool for fields and also for gravity.

Ossining, USA
August 2024

John Rider Klauder

A handwritten signature in black ink, reading "John R. Klauder", is placed on a light brown, irregularly shaped background that resembles a piece of paper or a stamp.

Preface

The summer of 2024 my wife Laure and my daughter Alice and myself decided to make a visit to Prof. John Rider Klauder, at that time 92 years old, living in Ossining, NY, USA, with his youngest daughter Jennifer. Before that I just interacted with John through email exchanges or Skype. We had already written and published 11 papers together. I got initially in touch with John fortuitously. In 2020, my wife Laure had just solved (exactly analytically) the harmonic oscillator problem on the half line using affine quantization [1] when John contacted her congratulating for the nice progress done. In that occasion, my wife told John that her husband was also a physicist working on Monte Carlo methods. So John contacted me proposing a Monte Carlo simulation of the quantum Euclidean covariant relativistic scalar field theory with a φ^4 potential in $3 + 1$ dimensions treated with affine quantization in order to see whether it would continue to be plagued by the triviality that appears when one treats it with canonical quantization. This brief book tells about the story of our 11 publications that stemmed from our collaboration and interactions through emails and voice messages exchanges, before we finally met in NY. John himself proposed the writing of the book the very last day of our stay in Ossining.

The book is a complete, coherent, organic, narrative, and possibly clear account of the 11 publications in collaboration with John from 2020 to 2024 which originated from John idea of trying to understand numerically through path integral Monte Carlo and possibly find a solution to the triviality problem with, for example, the φ^4 scalar field theory in $3 + 1$ spacetime dimensions when canonical quantization is used to describe it. This triviality issue constitutes the core of the book and it is given account, especially in the last section of the last chapter. The first chapters discuss instead the quantization procedure alternative to the canonical one, called “affine”, which will prove very useful where and when the canonical one fails.

In the book, we try to give derivations and proofs of any statement in a simple way accessible to any graduate student in physics or mathematics which we hope could benefit from it.

John used to give nicknames to the various paper he or we would compose. For example, he gave the name “killer paper” to Ref. [2] and as soon as he completed

successfully the tour de force on the commutation relations leading to the final result¹, he wrote me an email with subject “I did it!” and in the body after the main text he wrote “P. S. I named this paper ‘killer’ because of the difficulty in dissecting the affine kinetic term!”. As another example, the unpublished paper which is summarized in Sect. 2.7, he used to call the “zero paper”. In particular, this paper was written by me under his dictation through mp3 voice messages that he used to email me after he started having severe vision problems which would not allow him to work on his iPad, his window towards the physics community. John used to have brilliant ideas. Once he had the following great editorial idea: We had three papers ready named “killer-1,2,3”. I prepared “killer-1” and he prepared the other two. On 17 November 2021, he wrote me:

If you soon finish killer-1, please don’t send it to arXiv just yet. I am trying to get my preferred listing, and I am trying an experiment. I submit killer-2 first, you submit killer-1 next, and then I submit killer-3. These should be close in time so that they will be listed close together in arXiv’s lists.

To arrange all that I need you to offer times of day that could make it work for you. In my case, I am only using an iPad, which takes a bloody long time to submit because it is not a real computer and arXiv, as I found out, does not fix the system for non-computers, probably to keep some idiots away.

My son-in-law, who helps me submit my papers, might be present on Saturday in my morning if you could be available in your afternoon on Saturday, November 20. My 10 a.m. might work for your 4 p.m., for example. I need to make sure that my side can work all this tonight when he comes home from work. I will let you know soon.

We did the simultaneous submission on 20 November 2021 but unfortunately the experiment failed miserably because the archive moderators first put the three preprints on hold and then removed them all together. On 21 November 2021 John wrote me “My God they have removed killer-3 from arXiv altogether! Yes, some topics are repeated, but the breath of killer-3 was never larger and clearer. I am not happy!”

Meeting John in Ossining has been an extraordinary experience. He talks very slowly and you should also talk very slowly and clearly, possibly in good English without an Italian accent, if you want him to understand you. Otherwise, the kind daughter Jennifer would serve as an interpreter. He just came out of some vision problems which did not stop him from working at new manuscripts which he would dictate to me through voice messages. He moves slowly with some supports (also shown in the Photograph 1), has very little memory but is a tireless worker, especially when it comes to physics and mathematics. I think that he should be taken as an example for how much important can be to have a passion in life. He told us about many anecdotes like when he was a good table-tennis player, or when he met Einstein just before his death, or when he tried to repeat Galileo experiment from the top of Pisa leaning tower during one of his trips to Italy.

It has been a pleasure to meet John family with my family. In the Photograph 1, you can see us at a welcome dinner in the Henry Gourdine park on the Hudson river.

¹ By the way the final result was wrong by a factor 2 as I pointed out.

I would like to thank Jennifer and her husband Dustin for making the visit to Ossining possible and lively and for helping in communicating with John once there. I would like to thank Prof. Heinrich Leutwyler, who has been the first Ph.D. student of John, for many illuminating and profound email discussions on field theory and its role in the physics of the Standard Model. But also for proposing the calibration of my “numerical telescope” in producing Fig. 7.1 for the two-point function. Even if he never really showed himself fully convinced by the usefulness of AQ many of our discussions resulted in the realization of the content of Subsect. 7.3.3 of this book. Last but not least, I would like to thank my wife for being the initial link to this collaboration and the whole matter.

Trieste, Italy
August 30, 2024

Riccardo Fantoni

On 25 October 2024, the family of Prof. John R. Klauder has informed us of his death, which occurred on 24 October. We remember him as a great scientist, a man of culture who loved music, full of humor, grace, and kindness. His spirit of generosity, open-minded intellectual attitude, and keen intelligence guided him to the solution of intricate issues. He embodied a rare blend of rigor, creativity, and broad scientific knowledge that spanned mathematics, physics, and beyond. He was 92 years old. He said that nine was his favorite number and that he would pass away at 99 years old. I hope that the seed he planted in me will grow and flourish. We will miss him. May he rest in peace.

Initially, the book had John as coauthor and the idea was to prepare a SpringerBrief of 50 pages. At some point, Springer asked me to write a StandAlone volume of up to 100 pages. Now that John passed away, Springer asked me to remove John’s name from the authors. The alternative would have been to go through complicated legal matters keeping track of the beneficiary/legal guardian of the deceased author who would have had to sign the contract.

John most probably could not read the first four sections of Chaps. 2, 3, and the second section of Chap. 7 which were added and sent to him just before he passed away. When the previous portions of this Preface were written, he was still alive and therefore I don’t refer to him in the past over there.

John use to believe three things: i. nothing is new; ii. everything is related; iii. nobody cares.

Trieste, Italy
October 25, 2024

Riccardo Fantoni

This book is an attempt to describe the collaboration between me and Prof. John Rider Klauder from 7 October 2020 to 9 October 2024, just 15 days prior to his death. I have been probably his or one of his last students even if my age is not anymore that of a student. But I am glad to say that I never ended being a student and Prof. Klauder has been my last “maestro” in field theory, among others like Prof. Adriano Di Giacomo from the physics department of the University of Pisa, Italy, and Prof. Robert Leigh from the department of physics of the University of

Illinois at Urbana/Champaign, in the field of relativistic quantum mechanics, my first master advisor Prof. Mario Pio Tosi from the Scuola Normale Superiore di Pisa, Italy, my second master advisor Prof. David Matthew Ceperley from the National Center for Supercomputing Applications of the University of Illinois at Urbana/Champaign, and Prof. Bernard Jancovici from the laboratory for theoretical physics of the University of Paris Sud at Orsay, France, in the field of the electron gas, and Prof. Stuart Shapiro from the University of Illinois at Urbana/Champaign in the field of cosmology, gravitation, and compact objects in the Universe.

I received the first email message from John on 7 October 2020. It stated the following:

Dear Sir,

Classical versions of all covariant scalar models with positive interactions admit acceptable solutions, but some models will lead to divergences when trying to solve them when using canonical quantization. The problem deals with covariant scalar fields with power law interactions. The Euclidean time version of the action functional is then given, with $\varphi(x), x \equiv (x_0, x_1, x_2, \dots, x_s)$ for s spatial dimensions and $n = s + 1$ for the number of spacetime dimensions, and the complete action functional is given by

$$\int \left\{ \frac{1}{2} \left[\left(\sum_{j=0}^s \partial \varphi(x) / \partial x_j \right)^2 + m^2 \varphi(x)^2 \right] + g \varphi(x)^r \right\} d^n x$$

where g is the interaction term coupling constant and $r = 4, 6, 8, 10, \dots$ is the power of the interaction term. This model includes the standard relativistic scalar models. MC studies in 1982 showed that these models were correct for $r = 4$ and $n = 3$ but when $r = 4$ and $n = 4$ they led only to free models, as if $g = 0$, and this was confirmed later by analytic studies and that even became simply free models when $r = 4$ and $n > 4$ which includes non-renormalizable models as well. I can send you the 1982 MC paper if you like.

All of the above story used canonical quantization procedures, which then failed when $r \geq 2n/(n - 2)$. I believe that affine quantization (which Laure is now using) will solve those problems where $r \geq 2n/(n - 2)$. The 1982 paper provides a good background, but needs to apply a different set of discrete lattice approximations that are suggested by affine and not by canonical quantization. I have published such lattice suggestions that I can send you as well. While $r = 4$ and $n = 5$ is a non-renormalizable model, it involves too much computer time as well, so I am suggesting $r = 8$ or 10 and $n = 3$ which should be much easier to prove the principle. You might even like the article JHEPGC 6, 656–661. <https://doi.org/10.4236/jhepgc.2020.64044> [“An Ultralocal Classical and Quantum Gravity Theory”], which you need to use PDF to see the paper body.

I would be happy to send you additional material if you would be interested.

John Klauder

Followed an exchange of roughly 1000 emails received from his google address “john.klauder@gmail.com”

and 110 emails from his institutional address

“klauder@ufl.edu”

and all this in just four years!. Much more than with my two Ph.D. advisors from my two different Ph.D. in Physics in Urbana, Illinois and in Trieste, Italy in 30 years.

John has been extremely, extraordinarily, tirelessly active till the very end. The last message I received from him was on 9 October 2024 on occasion of the acceptance on Accademia Quantum of our last paper together and it said like so:

Bravo! You've done a great addition and I Suit. you. John.

We published 10 papers together on how Affine Quantization can help solving the triviality problem which plagues quantum (Euclidean) relativistic scalar field theories which would otherwise be inconsistent with the existence of scalar particles.

His first Ph.D. student, Heinrich Leutwyler from Bern, suggested the simulation of the non-interacting ($g \rightarrow 0$) purely Gaussian theory with my Path Integral Monte Carlo so that one could compare the numerical results with the analytically exact ones for the two point correlation function [Fantoni R. and Klauder J. R., "Monte Carlo evaluation of the continuum limit of the two-point function of the Euclidean free real scalar field subject to affine quantization", J. Stat. Phys. 184, 28 (2021)] [3].

The idea of writing a book came to John when we visited him on the summer 2024 from 29 July to 12 August, in Ossining, the old Sing Sing, where he was living with the family of his youngest daughter Jennifer. We started writing it together until his passing away on 24 October 2024 (Fig. 1).

Trieste, Italy
April 21, 2024

Riccardo Fantoni



Fig. 1 Dinner on the 3 August 2024 at “3 Westerly Bar and Grill”, 3 Westerly Road, Ossining, NY 10562. In front, Jennifer with the three years old daughter Riley. Behind, from left to right, Laure, John, and Dustin (Jennifer husband). On the back, from left to right, Alice and myself

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Competing Interests The author has no competing interests to declare that are relevant to the content of this manuscript.

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Chapter 1

Introduction



*Considerate la vostra semenza:
fatti non foste a viver come bruti,
ma per seguir virtute e canoscenza*

*Dante Alighieri
La Divina Commedia (canto XXVI inferno)*

Abstract In this chapter, we give a brief introduction to the book starting off in *medias res* with some details of the main topic covered that is Euclidean, Relativistic, Quantum, Scalar, Covariant, or Ultralocal Field Theory in Canonical and Affine Quantization.

The scope of quantum physics has expanded remarkably, as will be clear in this brief book. Many problems have new and novel results.

The basic rules of quantization were largely set around mid-(1920), and have changed very little thereafter. There are many problems that using those rules can lead to acceptable results, but there are many more problems that those rules are inadequate. As an example, the traditional harmonic oscillator, which is set on the whole real line, can be fully solved with the original rules. However, if the harmonic oscillator is set only on the positive real line, it cannot be solved with the old quantization rules despite the fact that it can be solved classically. Many problems that can be solved classically cannot be solved with old rules known as canonical quantization (CQ). Those procedures fail on nonrenormalizable examples which include certain relativistic scalar fields and Einstein's gravity.

A new quantization procedure, called affine quantization (AQ), has now been added to the old rules. This procedure is now about 30 years old. AQ is not well known and it deserves to be as strongly known as CQ. While CQ chooses the momentum, e.g., p , and the coordinate, e.g., q , to promote to quantum operators, AQ chooses what we call the *dilation*, namely $d = pq$.

We start slowly with simple models to appreciate what AQ is able to accomplish. Already, using Monte Carlo methods, several nonrenormalizable relativistic scalar

fields models have confirmed what AQ can do for them. Einstein's gravity is more complicated, but the rules of AQ offer considerably positive results [1].

When switching from quantum mechanics to scalar field theory [2] the position q becomes the scalar field $\varphi(x)$ where x denotes the spacetime coordinates. The momentum $p = \dot{q}$ becomes $\pi(x) = \dot{\varphi}(x)$ where we denote with the dot a time $t = x_0$ (or imaginary time in Euclidean field theory) derivative as usual. A brief example of the affine procedures, and a brief integration interval, considers the classical Hamiltonian $H = \int_{-1}^1 [\pi(x)^2 + |\varphi(x)|^r] dx < \infty$, with $r = 1, 2, 3, \dots$, then H can be finite if the integrand reaches infinity, e.g., $\pi(x)^2 = A/|x|^{1/4}$. This is proper mathematics, but the fields of nature should never reach infinity. Our solution introduces a new field, $\kappa(x) = \pi(x) \varphi(x)$. Now, $H = \int H(x) dx = \int [\kappa(x)^2 / \varphi(x)^2 + |\varphi(x)|^r] dx < \infty$. To represent $\pi(x)$, then $0 < |\varphi(x)| < \infty$, $0 \leq |\kappa(x)| < \infty$, and $H(x) < \infty$. Going to quantum field theory, while the field operator $\hat{\varphi}(x) = \hat{\varphi}(x)^\dagger = \varphi(x) \neq 0$, the momentum operator $\hat{\pi}(x)^\dagger \neq \hat{\pi}(x)$, then $\hat{\kappa}(x) = [\hat{\pi}(x)^\dagger \hat{\varphi}(x) + \hat{\varphi}(x) \hat{\pi}(x)]/2$, and after the scaling regularization, then the quantum Hamiltonian $\mathcal{H} = \int [\hat{\pi}(x)^2 + 2\hbar^2 / \hat{\varphi}(x)^2 + |\hat{\varphi}(x)|^r] dx < \infty$. Note that $|\hat{\varphi}(x)|^r < \infty$ for all x , and all r , $0 < r < \infty$, due to $0 < |\hat{\varphi}(x)| < \infty$ as well as $0 \leq |\hat{\pi}(x)| < \infty$!

The main actor of this short book will be Relativistic Covariant Euclidean Scalar Field quantization, nicknamed $(\varphi^r)_n$, where r denotes the power of the interaction term and $n = s + 1$ where s is the spatial dimension and 1 adds imaginary time. Models such that $r < 2n/(n - 2)$ can be treated by CQ, while models such that $r > 2n/(n - 2)$ are nonrenormalizable and trivial, leading to perturbative infinities, or, if treated as a unit, emerge as “free theories”. Models such as $r = 2n/(n - 2)$, e.g., $r = n = 4$, again using CQ also become “free theories”, which must be considered quantum failures. However, as remarked above, there exists a different approach called AQ that promotes a different set of classical variables to become the basic quantum operators and it offers different results, such as models for which $r > 2n/(n - 2)$, has been correctly quantized. For example, $(\varphi^{12})_3$ [3, 4]. Or models for which $r = 2n/(n - 2)$, has also been correctly quantized. For example, $(\varphi^4)_4$ [5–8].

Relativistic Ultralocal Euclidean Scalar Field quantization such that $r < 2$ can be treated by CQ, while models such that $r > 2$ and any $n \geq 2$ are trivial. However using AQ they remain “non-free theories”. For example, $(\varphi^4)_2$ [9].

AQ is a newer procedure that is qualitatively different than CQ. The difference is such that favored Cartesian classical variables [10] choose the basic quantum operators, while for AQ, the favored classical variables arise from a constant negative curvature. This is different from the constant zero curvature, i.e., a flat surface suitable for CQ. Indeed, it leads to AQ becoming a *partner procedure* and not a substitute for CQ, with each procedure appropriate for distinct sets of problems for them to treat. AQ has the very important property that it can only exist if there are *missing parts of space*, and that is shown by incomplete regions that still remain, e.g., if b is any number, $\varphi(x) > 0$, $|\varphi(x)| > 0$, $\varphi(x)^2 < b^2$, $\varphi(x)^2 > b^2$, etc. [11]. This may be used to describe correctly walls in quantum mechanics or even black holes [12].

When applied to quantum field theory (rather than quantum mechanics) AQ requires a regularization necessary to remove some subtle infinities through a proper

scaling transformation. This fact was initially overseen by us in our first publications during our collaboration [3, 5, 13]. But it has been taken properly into account at a later stage [4, 6, 8]. The secret to a valid CQ is remarkably simple. All you need is the addition of a single, fixed potential, which is not seen in the classical Hamiltonian, but it puts things in proper position elsewhere. This single potential is an additional “polynomial”-like self-interaction which is just $2\hbar^2/\varphi(x)^2$ as already mentioned above.

In order to assess the nontriviality of the various AQ Euclidean (in imaginary time τ) relativistic scalar field theories that we have been taking under exam we decided to proceed numerically rather than analytically. We then used the Path Integral Monte Carlo (PIMC) method to simulate the renormalized properties of the corresponding quantum lattice field theory, like the mass and the coupling constant. We were then able to study the renormalized coupling as a function of the bare mass, the bare coupling constant, and the spacetime lattice spacing. Our aim has been therefore to numerically prove that the renormalized coupling does not tend to zero as the lattice spacing is chosen smaller and smaller in order to approach the continuum limit, for some or any value of the bare coupling (and mass). We used periodic boundary conditions of the field around the finite spacetime simulation box in order to simulate an infinite spacetime, whereas the field is allowed to be any real number. The field path is a closed loop on an n -dimensional surface of an $(n + 1)$ -dimensional β -cylinder, with $\beta = 1/k_B T$ and k_B Boltzmann constant and T absolute temperature, so that $x_0 = ct \in [0, \beta[$ and c light’s speed constant. We will use natural units $c = \hbar = k_B = 1$ in all our simulations.

The book is an attempt to present the outcome of our collaboration on these issues as a coherent “whole”. We do this by giving proofs of any statement presented so that the book should be considered self-contained as much as possible. We hope that the book will become a useful reference tool for those graduate students or more generally for those mathematics or physics researchers who aim to dive deep into the still unsolved problems of the Standard Model (and especially the Higgs sector) or of Quantum Gravity.

The book is made of three introductory chapters and four main chapters:

In the first introductory chapter (Chap. 2), we introduce the problem of triviality of the φ^4 Relativistic Euclidean Scalar Quantum Field Theory in four spacetime dimensions and how it can be overcome with AQ. In the second introductory Chapter (Chap. 3), we describe the Higgs boson and the spontaneous symmetry breaking mechanism. In the third introductory Chapter (Chap. 4), we introduce the problem of Black Holes in Quantum Gravity and how it can be overcome with AQ.

In the first main Chapter (Chap. 5), we review the three main quantization procedures available in enhanced quantization (EQ) [14] and we learn how to quantize selected problems. In the second main Chapter (Chap. 6), we present the quantum relativistic Euclidean real scalar field theories of interest as treated through CQ and AQ, the scaling regularization necessary in AQ is discussed, and the applications to a restricted field space are treated [11]. In the third main Chapter (Chap. 7), we describe the path integral Monte Carlo method used to study the various CQ and AQ field theories previously introduced and present some of the numerical results

obtained in our computer experiments. In the fourth main Chapter (Chap. 8), we present the quantum relativistic Euclidean complex scalar field theory describing the Higgs Mexican hat system as treated through CQ and AQ, the scaling regularization necessary in AQ is discussed, and the numerical results from our path integral Monte Carlo computer experiments are discussed.

The experienced researcher may skip the first four sections of Chap. 2, all Chap. 3, and the last two sections of Chap. 5.

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Chapter 2

Triviality of Four-Dimensional φ^4 Theory on the Lattice



*“Guardaci ben! Ben son, ben son Beatrice.
Come degnasti d’accedere al monte?
non sapei tu che qui è l’uom felice?”*

*Dante Alighieri
La Divina Commedia (canto XXX purgatorio)*

Abstract In this chapter we introduce the problem of Triviality of the φ^4 Relativistic Euclidean Scalar Quantum Field Theory in four spacetime dimensions and how it can be overcome with Affine Quantization. How Affine Quantization offers the mathematical rigor necessary to prove the existence of Scalar Particles. The importance of infinities and of the number zero. The importance of the instrument of the Numerical Experiment which through the Monte Carlo method can solve exactly but numerically a Lattice Field Theory.

One of the most important ideas in field theory is the concept of particle mass generation by spontaneous symmetry breaking. This symmetry breaking is often produced by the introduction of a scalar field. This new field may interact with itself (via a φ^4 coupling) so as to produce a ground state for the theory which lacks a symmetry of the Hamiltonian. Gauge particles propagating in the asymmetric vacuum appear to be massive, and the underlying theory remains renormalizable. However such an assumption may not be correct. Many analytical and numerical works show that at least pure φ^4 field theory is “trivial” or noninteracting in four dimensions. So that, if the theory does not interact, its (nonexistent) interactions cannot break the symmetry of the vacuum, and gauge particles cannot acquire a mass through this mechanism. If this triviality is confirmed, it is fair to question the whole idea of symmetry breaking by elementary scalars. In this case the standard model might be a low energy effective model of a more complete theory. Although the situation with the standard model is not yet fully clear theoretically, still requiring a clear assessment of the Higgs mass bounds and prediction, it has been now proved experimentally that the Higgs scalar particle does exist. Some of the material of this introduction and of Sects. 2.1–2.4 was extracted from Ref. [1] Copyright @ Scholarpedia 2014.

Even if Euclidean quantum field theories are formally defined by their Hamiltonian density, except some rare toy models solvable analytically, to extract physical predictions is necessary to study the problem numerically. The theory should then be regularized at short distance by introducing an ultraviolet (UV) cutoff a which represents the lattice spacing. Then measurable values emerge from suitable renormalized correlation functions in the *continuum limit* where this cutoff is removed.

A quantum field theory is called *trivial*, if this continuum limit leads to a non interacting renormalized theory despite the presence of interaction terms in the bare Hamiltonian. Of course it is possible that such a theory can still describe Nature if there is a range of its free parameters such that:

- interactions are strong enough to be experimentally observed;
- finite cutoff effects cannot be observed and are negligible at accessible momenta.

It could happen that the effects of the cutoff are invisible on a certain limited range of scales to a certain precision. Such an *effective field theory* is expected to be finally replaced by a more comprehensive theory valid beyond the restricted range. This could happen, for example, in the elementary scalar “Higgs” particle (see Chap. 3). In the theoretically elegant Higgs mechanism, the interactions of elementary scalars are used to generate gauge boson masses in a quantum field theory. However, strong evidence suggests that at least a pure φ^4 scalar field theory is trivial or noninteracting. This triviality also affects theoretically more complicated systems such as the standard model of the weak interaction even if it has now been discovered experimentally the Higgs particle. On the other hand, the presence of gauge and fermion fields, that has been superseded and extended by the Weinberg-Salam theory, can rescue a pure scalar theory from triviality. Phenomenological constraints, such as a bounded or even predictable Higgs mass, may then be implied even theoretically [2].

Specifically we will worry about the simplest quantum field theory of a single real scalar field $\varphi(x)$ attached to each point of n -dimensional euclidean spacetime. We will then choose $n = 4$ and analytically continue to Minkowski spacetime. The most important class of observables is given by the correlation functions defined through the following functional integrals:

$$\langle \varphi(x_1)\varphi(x_2)\cdots\varphi(x_k) \rangle = \frac{1}{\mathcal{Z}} \int \varphi(x_1)\varphi(x_2)\cdots\varphi(x_k) \exp(-S[\varphi]) \mathcal{D}\varphi(x), \quad (2.1)$$

with the action

$$S[\varphi] = \int \left\{ \frac{1}{2}[(\nabla\varphi)(x)^2 + m^2\varphi(x)^2] + g\varphi(x)^r \right\} d^n x, \quad (2.2)$$

where r is an even number and $\mathcal{Z}$ is the normalizing partition function achieving $\langle 1 \rangle = 1$. This formal definition requires a regularization. There are two main strategies to define and evaluate functional integrals:

- Perturbative approach: the weight $\exp(-S[\varphi])$ is expanded in powers of g and then the integral becomes a sum of Gaussian (quadratic in the exponent) expectation

values of polynomials of φ . Such integrals can be evaluated formally and lead to the famous Feynman diagrams. The individual terms diverge and still need regularization. There are many ways to do this within perturbation theory, as for example continuing to non-integer n , or by modifying the action to suppress the large momentum components in φ . Note the unsatisfactory aspect of mixing up approximation and definition in this approach.

- Nonperturbative lattice approach: The infinite spacetime continuum is replaced by a finite lattice that has to be large and dense enough. Then the functional integral can be rigorously defined as a limit of a sequence of ordinary integrals. In the lattice formulation, various expansions as well as other numerical methods to approximate the high-dimensional integrals may be applied with characteristic domains of validity. Most notably this includes Monte Carlo simulation (see Chap. 7).

Our aim is to discuss structural properties of the φ field theory at arbitrary values of its free parameters m and g including such values where the series expansion in g may not give the true answer. We will then mainly focus on the lattice definition, even if inspiration from perturbation theory is still essential to design definitions and parameterizations.

2.1 Symmetric Phase

Consider a cubic lattice with spacing a and periodicity L in each direction (hypertorus). There are $(L/a)^n$ points or sites x , and the functional integral $\int \mathcal{D}\varphi \dots$ is defined as independent integrations over the entire real line of $\varphi(x)$ for each x . In the definition of the action S we replace

$$\int d^n x \dots \rightarrow a^n \sum_x \dots, \quad \nabla_\mu \varphi(x) \rightarrow [\varphi(x + e_\mu) - \varphi(x)]/a, \quad (2.3)$$

where e_μ is a vector of length a in the $+\mu$ direction with $\mu = 0, 1, 2, \dots, s$.

An important observable is the two-point correlation function $\langle \varphi(x)\varphi(y) \rangle = G(x - y)$ where x, y must be lattice sites, of course, and translation invariance on the hypertorus makes G depend on $x - y$ only. We can pass to momentum space (see Sect. 7.3)

$$\tilde{G}(p) = a^n \sum_x e^{ip \cdot x} G(x), \quad p \in \left(\frac{2\pi}{L} \mathbb{Z} \right)^n, \quad (2.4)$$

where the components p_μ on the hypertorus are integer multiples of $2\pi/L$. In the free theory ($g = 0$), one can now perform the finite dimensional Gauss integrals and obtains the free propagator

$$\tilde{G}(p) = \frac{1}{\hat{p}^2 + m^2}, \quad \hat{p}_\mu = \frac{2}{a} \sin(ap_\mu/2), \quad (2.5)$$

which, in position space, corresponds to an asymptotic decay of $G(x)$ proportional to $\exp(-m|x|)$ up to power corrections. The physical scale that is thus encoded in the correlations is the correlation length $\xi = 1/m$. In this case the lattice is considered large and dense (sufficiently fine resolution) if $a \ll \xi \ll L$ holds. One may now consider the

- thermodynamic limit $L/\xi \rightarrow \infty$,
- continuum limit $a/\xi = am \rightarrow 0$.

They may be taken in either order (or even simultaneously) and in both cases the extrapolation leads to a diverging number of lattice sites. Renormalization theory suggests that these limits exist in the interacting theory with $g > 0$. Even if it is necessary to replace the bare parameters m, g with other (renormalized) ones.

For example, all experiences from perturbation theory suggest that in the limit of small momenta, the two-point function becomes

$$\tilde{G}(p) = \frac{Z}{\hat{p}^2 + m_R^2}, \quad \hat{p}^2 \rightarrow 0, \quad (2.6)$$

where the dimensionless quantities Z, am_R , extracted from the limiting behavior of $\tilde{G}(p)$ at small p (or $G(x)$ at large $|x|$), are nontrivial but well defined functions of am and g . The decay of correlations is now characterized by $\xi = 1/m_R$. The renormalized mass of the scalar particles described by this quantum field theory is essentially given by m_R ,

$$m_R^{-2} = - \left. \frac{d}{dp^2} \ln \tilde{G}(p) \right|_{p=0}, \quad (2.7)$$

in the continuum, where $\tilde{G}(p)$ is the renormalized two-point function in momentum space. See Sect. 7.3.1 for the lattice version of m_R . While the parameter m no longer has a direct physical meaning.

A physical measure of interaction is related with scattering cross sections of the particles. For certain processes they are determined by four point correlations. This leads to a possible definition of a renormalized coupling constant g_R by (see Sect. 7.3.2)

$$g_R = 3 - \frac{\langle \tilde{\varphi}(0)^4 \rangle}{\langle \tilde{\varphi}(0)^2 \rangle^2}, \quad \tilde{\varphi}(0) = a^n \sum_x \varphi(x). \quad (2.8)$$

This g_R has a number of important properties:

- g_R is dimensionless and non-negative. This a result due to Joel Lebowitz (the so called Lebowitz inequality),
- $\lim_{g \rightarrow 0} g_R = 0$ as the numerator vanishes for Gaussian measures,
- the thermodynamic limit exists smoothly and is assumed to have been taken from now on with the situation hence being: $0 \leq am_R \ll 1$, $m_R L \rightarrow \infty$.

The continuum limit for this model amounts to tuning the bare parameters am , g to arbitrary values (where the integrals exist, however) such that $am_R = a/\xi$ goes to zero. Generically, we might expect this to happen on a curve in the (am, g) plane [including the free point $(0, 0)$], and different points on this ‘continuum curve’ may correspond to different physical interaction strengths g_R in the continuum theory. Note that renormalized continuum correlations emerging in the limit may still depend on m_R which thus can survive as the physical scale. This rather generic picture is essentially correct for $n = 2, 3$, but in $n \geq 4$ one encounters the phenomenon of triviality: $g_R \rightarrow 0$ whenever one tunes for the continuum limit $am_R \rightarrow 0$. Thus only free non interacting theories are reached in the strict continuum limit.

This kind of triviality of lattice φ^4 theory has been rigorously proven for $n > 4$ while for the most interesting borderline case $n = 4$ we have only partial results but very strong evidence from numerical simulations. Interestingly perturbation theory predicts triviality as long as the truncated expansion in g_R is justified. Note that this is entirely possible without g being small. However, there remains the logical possibility that a nontrivial continuum limit exists with some g_R where perturbation theory is simply irrelevant. It is this gap which one tries to close by numerically exact numerical experiments.

2.2 Broken Symmetry Phase

So far it was tacitly assumed that $G(x)$ decays to zero at large distance. If we imagine a negative value of $m^2 < 0$, then, for constant fields, S is an integral over a double well shaped density with minima at $\varphi(x) = \pm \bar{\varphi}$ with $\bar{\varphi}^2 = -m^2/(4g)$. Then in perturbation theory, for $n > 1$, the dominant contributions to the path integral come from fluctuations around one of these minima (rather than the zero field as before) which is picked by the spontaneous breaking of the symmetry $\varphi \rightarrow -\varphi$. This leads to a non-vanishing constant one point function $\langle \varphi(x) \rangle$ and particles are associated with the small fluctuations around it. From the subtracted two-point function (see Chaps. 8 and Sect. 7.3.3)

$$K(x) = \langle \varphi(x)\varphi(0) \rangle - \langle \varphi \rangle^2, \quad (2.9)$$

one may now extract m_R and Z in the same way as before. Now perturbation theory is set up after shifting the integrations by $\bar{\varphi}$. From the quadratic part of the shifted action one reads off the leading order result $m_R^2 = -2m^2 + \dots$.

2.3 Trivial and Effective Theories

A trivial theory in the continuum limit can still be useful as an effective theory if one does not reach the mathematical limit and does not remove completely the lattice (or other UV cutoff). It is possible that a sufficiently small value of am_R allows to find good agreement with the experiment if the parameter values are such that the interaction is big.

Often, historically, one realizes that theories undergo modifications which in turn give rise to their extension. The spirit of looking for the theory with the largest domain of validity resembles the one of allowing for an effective theory from a lattice theory. From this point of view triviality can even be seen as a plus rather than a minus or a defect. Of course one has to keep in mind that even if one can reproduce the experimental values with an effective theory this does not mean that the theory so constructed is universal at all. In fact it is often the case that one encounters non universal properties which differ from one (unphysical) regularization to another.

2.4 Numerical Results

Numerical experiments aim to support the triviality conjecture in $n = 4$ predicted by perturbative renormalization group theory near a critical line of the phase space.

In exact numerical simulations one has to worry with two sources of errors related to the three length scales a, ξ, L . On a computer the number of sites L/a in each direction is limited. In order to approach the renormalization group behavior we have to worry first about the continuum limit fixing L/ξ to some order one value and achieving a larger $\xi/a \gg 1$ and then about the thermodynamic limit choosing $L/\xi \gg 1$. One usually refers to this last source of error due to working with a finite L as the finite-size. Moreover in a Monte Carlo simulation one has also to master the unavoidable statistical error. Triviality is considered an ultraviolet renormalization effect and our tests conducted along these lines have supported the triviality scenario up to now.

As discussed in this chapter, strong evidence suggests that a theory which only includes Higgs particles (see Chap. 3) is “trivial” or noninteracting. Should this triviality persist when the Higgs is “hitched to everything else” in the standard model, then the standard model scenario is in trouble. It would then be fair to ask if a real “Higgs particle” should exist, or whether this putative elementary scalar is instead just an invisible metaphor for a more complicated mechanism. The obvious question to ask—what this new mechanism may be—is not as obviously answerable. A more informative set of possibilities does, however, exist if the Higgs sector of the standard model (or indeed of any realistic Higgs model) is nontrivial. In this case it is likely possible to calculate upper bounds upon the Higgs mass or even to predict its value. The requirement that the theory be nontrivial thus can imply phenomenological constraints on the theory. By contrast, a naive semiclassical analysis of the scalar

sector of the standard model does not yield any information on the Higgs mass. It is evident that the question of the triviality of Higgs models is of more than philosophical interest. Progress is being made in the understanding of triviality and its implications for elementary particle phenomenology. Much remains to be done, however. Although techniques such as the analysis of lattice gauge theories by the Monte Carlo renormalization group may well hold the key to the riddle of triviality, the final answers are not yet known. We therefore conclude with the question: Can elementary scalar particles exist?

2.5 Freedman, Smolensky, and Weingarten

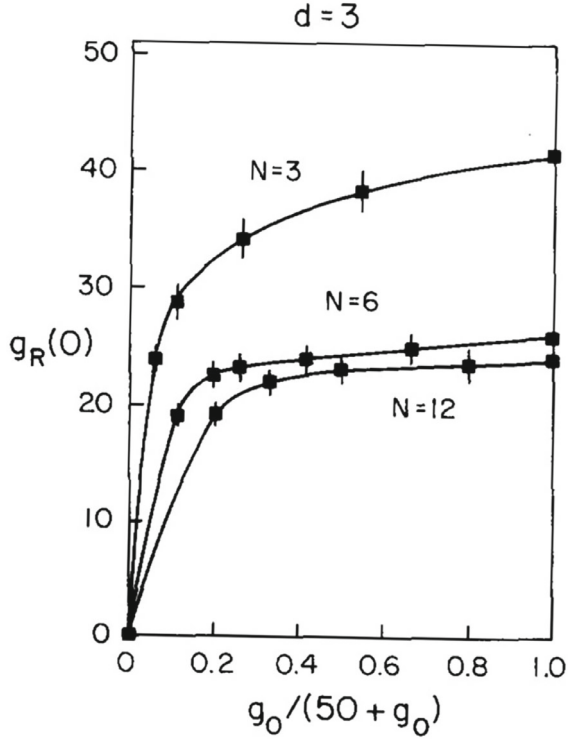
A landmark calculation of this form was performed by Freedman, Smolensky, and Weingarten [3]. This was also the seed that prof. Klauder proposed to me at the very beginning from which all of our following collaboration would stem.

Using standard Monte Carlo techniques, the Fourier transform $\tilde{\varphi}$ is computed. According to the philosophy outlined above, the lattice spacing a is sent to zero while the volume $L^n = (Na)^n$ is kept fixed. In practical terms this means that a series of measurements are made upon a sequence of lattices with N taking increasingly larger values (so that the lattice spacing a is progressively smaller). For each value of N , the bare mass m is adjusted until the renormalized mass equals a certain value. The value $m_R = 3.63$ (with estimated error of a few percent) was chosen by these authors. This choice of m_R was motivated as a compromise between the simultaneous requirements that the volume be large and the lattice spacing be small in units of m_R^{-1} .

Once this tuning of m was achieved, the value of g_R was evaluated as a function of the bare quartic coupling $g = g_0$. These results are shown in Figs. 2.1 and 2.2 for $r = 3$ and 4. The contrast between the two cases is evident. In three dimensions (Fig. 2.1) g_R appears to approach a nonzero limiting value as the lattice spacing decreases. This is as expected, for in three dimensions $(\varphi^4)_3$ field theory is nontrivial. On the other hand, in four dimensions a trivial theory is anticipated. Consonant with this expectation, g_R approaches zero uniformly in this limit (Fig. 2.2). The optimism generated by the apparent ease of producing these results must be tempered with realistic judgment, however. First, it is well to remember that a complete error analysis of these and other related results [4–8] is lacking. Errors arise in such calculations from both systematic effects (like the trial and error enforcement of the constant renormalized mass constraint and the finite volume of the lattice) and statistical effects (critical slowing down).

Nevertheless it is exciting to consider the possibilities which open up when these numerical computations are taken seriously. For instance, one novel result of Ref. [5] was the finding that the two-point function was equal to the free field correlation function. These conclusions imply that the renormalized theory is at best very weakly interacting. Simulations in the broken symmetry phase of the theory [7] yield results which also are consistent with the triviality of φ^4 field theory in four dimensions.

Fig. 2.1 The zero momentum coupling constant g_R as a function of the bare coupling constant ratio $g_0/(50 + g_0)$ for $(\varphi^4)_3$ on lattices of size $N = 3, 6$, and 12. Redrawn from Ref. [3]. Their d is our $n = s + 1$, the spacetime dimensions



2.6 The Secret to Fixing Incorrect Canonical Quantizations

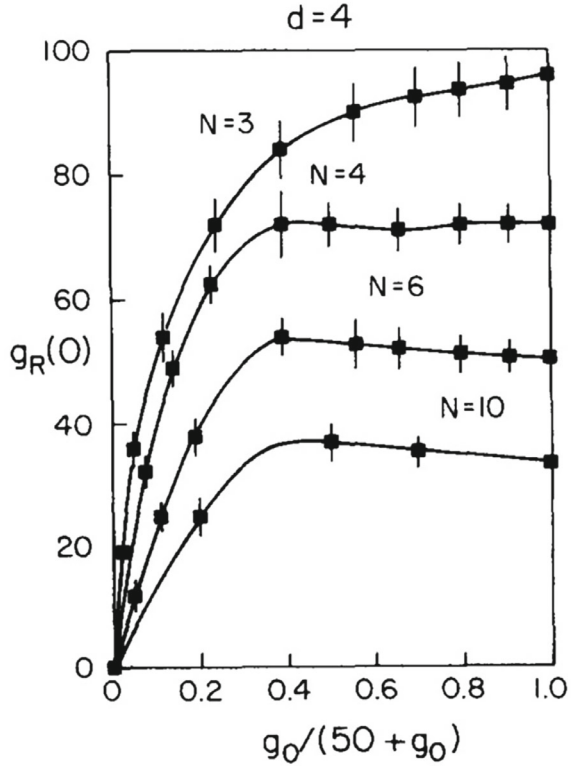
There have been many models¹ with the same ‘illness’ as that of φ_4^4 [1, 3, 10–14]. The secret to a valid canonical quantization (CQ) is remarkably simple. All you need is the addition of a single, fixed potential, which is not seen in the classical Hamiltonian, but it puts things in proper position elsewhere. This single, additional, potential is just $2\hbar^2/\varphi(x)^2$. Give it a try-out on the model φ_4^4 and see for yourself! You can also give it a new try with φ_4^8 and be surprised! **That additional ‘potential’, put just after $\hat{\pi}(x)^2$, is all you need to use.**

2.6.1 Amazing Results by Just Removing $\varphi(x) = 0$

The special $\hbar$ -term has arisen from the fact that $\varphi(x) = 0$ has been removed, which then means that the momentum is no longer self-adjoint. The next step leads to introducing $\hat{\kappa}(x) = [\hat{\pi}(x)^\dagger \varphi(x) + \varphi(x) \hat{\pi}(x)]/2$, and with scaling can lead to become

¹ Much of the material in this section is extracted from our Ref. [9].

Fig. 2.2 The zero momentum coupling constant g_R as a function of the bare coupling constant ratio $g_0/(50 + g_0)$ for $(\varphi^4)_4$ on lattices of size $N = 3, 4, 6$, and 10 . Redrawn from Ref. [3]. Their d is our $n = s + 1$, the spacetime dimensions



$$\pi(x)^2 = \kappa(x)^2/\varphi(x)^2 \rightarrow \hat{\kappa}(x)\varphi(x)^{-2}\hat{\kappa}(x) \Rightarrow \hat{\pi}(x)^2 + b\hbar^2/\varphi(x)^2, \quad (2.10)$$

and the factor $b = 2$ has been chosen to fit our particular problem. **Observe that choosing $\varphi(x) \neq 0$ has permitted introducing the ‘polynomial’-like term $2\hbar^2/\varphi(x)^2$.**

2.6.1.1 Understanding How Scaling Works

Initially $\hat{\kappa}(x)\varphi(x)^{-2}\hat{\kappa}(x) = \hat{\pi}^2 + \hbar^2\delta(0)^{2s}/\varphi(x)^2$, here $\delta(0)$ is Dirac’s special function, where $\delta(x) = 0$ for all $0 < |x|$, while $\int \delta(x) dx = 1$ which leads to $\delta(0) = \infty$. Now our ∞ is reduced to $a\hbar^2 W^2 < \infty$, and W will be sent to ∞ later on.

This now becomes $\hat{\pi}(x)^2 + a\hbar^2 W^2/\varphi(x)^2$. Next $(\hat{\pi}(x)^2 \& \varphi(x)^2) \rightarrow W(\hat{\pi}(x)^2 \& \varphi(x)^2)$. This leads to $W\hat{\pi}(x)^2 + a\hbar^2 W^2/W\varphi(x)^2$, and now a full multiplication by W^{-1} leads to the final result which is $\hat{\pi}(x)^2 + a\hbar^2/\varphi(x)^2$. Now W can be sent to infinity.

2.6.2 Selected Topics of Affine Quantization

A major feature of CQ is that $-\infty < q$ & $\varphi(x) < \infty$ either in quantum mechanics where q is position or in scalar field theory where $\varphi(x)$ is the field. It is that fact which affine quantization (AQ) overcomes by introducing a vast variety of parts of incomplete space, such as these retained space, $q > 0$, $|q| > 0$, $q^2 < b^2$, $q^2 > b^2$, etc. For quantum field theory, the most important change is that $\varphi(x) \neq 0$ **and now that equation has been fully removed.**

Observe, that CQ requires $0 \leq |\varphi(x)| < \infty$, while AQ seeks to find missing equations which shows that **a specific field value, namely, $\varphi(x) = 0$ is removed [15], or explained differently, now $0 < |\varphi(x)| < \infty$.**

2.6.2.1 An Introduction to AQ

Only AQ can correctly solve all examples that have missing space regions, and it can do it correctly only with remaining space examples.

There is something else that CQ can surely fail on, namely the example of the “Particle in a Box”, which is an example with missing space, and has been traditionally ‘solved’ using CQ. However, that very model can, and has, been correctly solved now by using AQ [14].

If you wish to read up on AQ, here are two examples where AQ has been well explained; see [14, 16].

There have been many models with the same ‘disease’ as that of φ_4^4 [1, 3, 10–14]. The secret to a valid canonical quantization is remarkably simple. All you need is the addition of a single, fixed potential, which is not seen in the texts, but it puts things in proper position elsewhere. This single, additional, potential is just $2\hbar^2/\varphi(x)^2$, alongside $\hat{\pi}(x)^2$. It is noteworthy that this potential forces $0 < |\varphi(x)| < \infty$ which leads to $0 < |\varphi(x)|^r < \infty$, and guarantees that almost all other potentials remain finite.

Give it a try on the model φ_4^4 and see for yourself! You can also give it a new try with φ_4^8 and be surprised! **That additional potential is all you will need.**

The secret to this magic has come from affine quantization [16].

2.7 A Modest Redirection of Quantum Field Theory Solves All Current Problems

Standard quantization using for example path integration of field theory models, includes paths of momentum and field reach infinity in the Hamiltonian density, while the Hamiltonian itself remains finite. That fact causes considerable difficulties. In this section, we represent $\pi(x)$ by $k(x)/\varphi(x)$. To insure proper values for $\pi(x)$ it is necessary to restrict $0 < |\varphi(x)| < \infty$ as well as $0 \leq |k(x)| < \infty$. Indeed that

leads to Hamiltonian densities in which $\varphi(x)^r$, where r can be even integers between 4 and ∞ . This leads to a completely satisfactory quantization of field theories using situations that involve scaled behavior leading to an unexpected, $\hbar^2/\hat{\varphi}(x)^2$ which arises only in the quantum aspects. Indeed, it is fair to claim that this symbol change leads to valid field theory quantizations.

Infinity is a difficult aspect of any issue in classical and quantum physics. Interestingly, this also infects zero as part of values that run between plus and minus infinity. It is evident that infinity as a symbol leads to $\infty + \infty = \infty$ as well as $\infty \cdot \infty = \infty$. It is evident here that zero follows the same procedure. Namely, $0 + 0 = 0$ as well as $0 \cdot 0 = 0$. It is noteworthy that zero was banned from using for 1500 years long, ago, but if a symbol, for example A , stands for an object which is specific, namely a brick or a tree or a screwdriver but these are unequivalent to each other having no screwdriver as a zero is just as saying that book equals zero and therefore book equal screwdriver equal zero. A field of nature, such as a particle of creation, is as unique as anything else and therefore its zero value deserves better treatment. In fact, if zero represents nothing then it could be that $\varphi(x) = 0$ also serves as nothing and $\varphi(x) = \pi(x) = 0$ leads to the fact that different kind of fields that appear are poorly labeled. A field $\varphi(x)$ can represent a particle of nature, but $\pi(x)$ we choose to use for the time derivative of $\varphi(x)$. $\pi(x) = 0$ with no wrong interpretation, but $\varphi(x)$ should not equal zero at all. Our current field theories would use $-\infty < \varphi(x) < +\infty$. In this case field theory has gone its happy way certainly classically but it really upsets things during quantization. One manner to be useful in eliminating $\varphi(x) = 0$ all together is to introduce a friendly new classical function. In particular, we introduce $k(x) = \varphi(x)\pi(x)$. $\varphi(x)$ we said can be zero and $k(x)$ then equals zero as well. But $\varphi(x) = 0$ when $\pi(x) = 300$ does not fit the physics of $k(x) = 0$. It is natural that we withhold any $\varphi(x)$ equaling zero, they are abandoned from our business and therefore we have correct $\varphi(x)$ and $\pi(x) = k(x)/\varphi(x)$ and have arranged to have $\varphi(x)$ withdrawn from our arithmetic if it is zero. Now why can that be useful.

Consider the field functions in a Hamiltonian density which are $\pi(x)$ and $\varphi(x)$ such as $\pi(x)^2$ and $\varphi(x)^2 + g|\varphi(x)|^r$ is a toy example for our analysis. It is a fact that when π and φ reach infinity in such a fashion that the integral Hamiltonian can still remain finite. In other words a finite Hamiltonian function can include density $\varphi(x)$ and $\pi(x)$ which reach infinity. Why would we want that? Because the quantization, most clearly in a path integration, has paths which actually reach infinity in such a slim way and therefore include fields that contribute to the Hamiltonian itself. **Nature should not reach infinity.** How can we take our fields into the density and retain them from ever reaching infinity. If that can happen, a very much should be more correct in its behavior than normally used.

We change variables in such a fashion that was having $k(x) = \varphi(x)\pi(x)$ and now use our toy Hamiltonian density our functions become $k(x)^2/\varphi(x)^2 + \varphi(x)^2 + g|\varphi(x)|^r$. It is clear that $\varphi(x) = 0$ is helpful here and helpful at infinity because if infinity of φ is allowed then $k(x)$ could not properly serve $\pi(x)$. Moreover we can have $|k(x)| < \infty$, but equal zero is fine, and since $|\varphi(x)|$ is also less than infinity, it follows that $|\varphi(x)|^r$ never reaches infinity as desired. Summarizing this paragraph it says that π and φ can completely substitute instead k/φ . There is complete confidence

that although the standard variables for classical theory don't want to reach infinity and do not, that means they are fully equivalent to our choice of the second version of the Hamiltonian density. Now however, we have a set of classical variables that are guaranteed to not reach infinity in the entire Hamiltonian density. Clearly it would seem that those variables deserve to become quantum variables. Our challenge now is to accept these two new variables $\hat{k}(x)$ and $\hat{\phi}(x)$, along with $\hat{\pi}^\dagger(x) \neq \hat{\pi}(x)$ we accept that and introduce $\hat{k}(x) = [\hat{\pi}^\dagger \hat{\phi}(x) + \hat{\phi}(x) \hat{\pi}(x)]/2 = \hat{k}^\dagger(x)$.

2.7.1 Wrestling with Infinities and Quantization

2.7.1.1 Nonrenormalizability in Canonical Field Quantization

In standard canonical quantization, we find the equation $[\hat{\phi}(x), \hat{\pi}(y)] = i\hbar\delta(x - y)$. Implicitly, that applies that $[\hat{\phi}(x), \hat{\pi}(x)] = i\hbar\infty$ which evidently leads to absolute value of $|[\hat{\pi}(x), \hat{\phi}(x)]| = \hbar\infty = \infty!$ In addition, while $\hat{\pi}(x)^2 + \hat{\phi}(x)^2$ is chosen as a simple toy model for Hamiltonian density. This has a domain of vectors that can be normalized. However the domain of those vectors will shrink if the expression has $|\hat{\phi}(x)|^{2+\epsilon}$ where $\epsilon > 0$. However if ϵ reduces to zero the domain does not recover itself therefore that can introduce complications. Another way to state that kind of problem is to chose $\hat{\pi}(x)^2 + \hat{\phi}(x)^2 + g|\hat{\phi}(x)|^r$ with $r > 2$. Once the g is positive, it determines the new domain, but if g goes to zero, the initial domain which is bigger than the case where g is positive does not return. Issues like that complicate conventional canonical field quantization. Initially, we now start a procedure that simplifies matters greatly.

2.7.1.2 Eliminating Infinities Through a Change of Variables and a Scaling

We have already found in classical formulation of the Hamiltonian density that fields could reach infinity conventionally, however in using the variables $\pi(x) = k(x)/\phi(x)$, can eliminate classical infinities in path integration. This is because our density contains $k(x)^2/\phi(x)^2 = \pi(x)^2$. Therefore $\phi(x)$ should not be zero or infinity in magnitude to complicate π itself while $k(x)$ cannot reach infinity again to not complicate π . In this section we treat the kinetic factor $\pi(x) = k(x)/\phi(x)$ as a term needed in the quantum Hamiltonian. We choose $\hat{\pi}(x)^2 = \hat{k}(x)[\hat{\phi}(x)]^{-2}\hat{k}(x)$ which has been discussed in several articles as a suitable quantum feature of the kinetic term in several papers already [14]. It is possible to change the term $\hat{k}\hat{\phi}^{-2}\hat{k}$ into $\hat{\pi}^2 + \hbar^2\infty/\hat{\phi}^2$ which now introduces infinities again. It is greatly noteful that the kinetic term has now increased itself in giving a "potential type term". That implies that the original kinetic term $\hat{\pi}^2$ has introduced as well a field potential albeit infinity. To obtain the equation there could be simply to take the following result somewhat reduced by introducing $\hat{\pi}^2 + a\hbar^2 W^2/\hat{\phi}^2$, where W will be sent to infinity fairly soon.

Now we do some rescaling in which we take $W\hat{\pi}^2 + W\hat{\phi}^2$. This modification leads to $W\hat{\pi}^2 + a\hbar^2 W^2/W\hat{\phi}^2$. It is clear now that all terms are proportional to W and therefore the final story will be taking the quantity $W\hat{\pi}^2 + a\hbar^2 W/\hat{\phi}^2$. That reveals the W . We then have a situation which leads to finally $\hat{\pi}^2 + a\hbar^2/\hat{\phi}^2$ which permits us to say the result can be any factor for the potential namely, $\hat{\pi}^2 + Z/\hat{\phi}^2$, in which Z is made of $\hbar^2$ so we can adjust a to be $Z = a\hbar^2$ and we require that $0 < Z < \infty$. This potential, $Z/\hat{\phi}^2$, is a kind of potential because is not possible to reduce Z back to zero in doing this quantization relation. It is only when quantum theory sends $\hbar \rightarrow 0$ to recover classical theory and then in that case Z would disappear.

2.7.1.3 Affine Field Quantization

So far in our story we begin to close up by establishing the essence of what we have said. If a classical mood for a classical Hamiltonian listed as $H_1 = \int \{[\pi(x)^2 + (\nabla\phi(x))^2 + m^2\phi(x)^2]/2 + g\phi(x)^r\} d^s x$ which represents relativistic classical Hamiltonian has difficulties especially when dealing with ϕ^4 which has seen multiple records using Monte Carlo studies that do not lead to acceptable answers. Indeed in the model $H_2 = \int \{[\pi(x)^2 + m^2\phi(x)^2]/2 + g\phi(x)^r\} d^s x$, which represents our ultralocal model, it will certainly fail, and has in fact done so, and done more poorly than the model H_1 . However that has been using canonical quantization. A new quantization procedure, called *affine quantization*, has been able to rigorously solve H_2 and H_1 automatically then. Indeed a respectable number of Monte Carlo studies have shown that using affine quantization can lead to very acceptable results for H_2 and H_1 . A complete story for both cases is well documented in Ref. [14]. Readers, who are interested in the details, can be made available in that strong article within archive. That article contains quantizations of field theory along with gravity and offers a very complete version of their being solved. For those readers, we hope you find whatever you will need to know.

In this book we will then show a simple switch of classical variables to represent $\pi(x) = k(x)/\phi(x)$. These variables all live below infinity in magnitude as well as field values must be greater in magnitude than zero. This procedure has been called upon to eliminate $\phi(x) = 0$ points of nature because zero can also complicate equations involved. As we have seen, removing $\phi(x)$ values when they are zero can remarkably help in the complete and correct quantization of common field theories.

2.8 The Number Zero Is Welcomed by Mathematics, but Physics Should Be Careful When Dealing With It

The number zero is happily used by mathematics, but not physics for various reasons. It should be incorrect to say that $\phi(x) = 0 = \gamma(x)$, when there are two, different, physical meanings, such as fields for two very different kinds of particles, etc. That

could lead to some kind of confusion in physics. In that case, it could even be necessary to **reject** using the zero number in certain expressions, and instead, at least try to ‘go around them’.

Do not forget [15] that the number zero was *banned* for 1,500 years, long, long ago!

There have been many models with the same ‘disease’ as that of φ_4^4 [11, 17]. The secret to a valid canonical quantization is remarkably simple. All you need is the addition of a single, fixed potential, which is not seen in the texts, but it puts things in proper position elsewhere. This single, additional, potential is just $2\hbar^2/\varphi(x)^2$, alongside $\hat{\pi}(x)^2$. It is noteworthy that this potential forces $0 < |\varphi(x)| < \infty$ which leads to $0 < |\varphi(x)|^p < \infty$, and guarantees that almost all other potentials remain finite.

The secret to this magic has come from affine quantization [16].

This example would consider integrations in which $\int_{-1}^1 |x|^p dx < \infty$ with $-1 < p < \infty$, would still get an identical result without needing $x = 0$. More importantly, the integral, $\int_{-1}^1 |\varphi(x)|^p d\varphi(x)$ gets an identical result without needing $\varphi(x) = 0$.

2.8.1 Why Removing Certain Zeros Can Be Important

Suppose you were dealing with two very different fields, $\varphi(x)$ and $\beta(x)$. Is the mathematical equation $\varphi(x) = 0 = \beta(x)$ physically correct? To satisfy both mathematics and physics, it would be far more correct if such ‘zero equations’ are *fully eliminated by removing them altogether*.

Not only would that be mathematically acceptable, but it could have a positive effect on other equations, such as $\int e^{-A/x^2 - Bx^2} dx$, which permits $x \neq 0$, or also said as $0 < |x| < \infty$. Of greater interest, $\int e^{-C/\varphi(x)^2 - D\varphi(x)^2} d\varphi(x)$, which permits removing $\varphi(x) = 0$, or also said as $0 < |\varphi(x)| < \infty$.

2.8.2 How Removing a Particular Zero Can Solve a Familiar Problem in Quantum Field Theory

The familiar φ_4^4 model, using canonical quantization, which did not get positive results stems from

$$\mathcal{H} = \int \left\{ \frac{1}{2} [\hat{\pi}(x)^2 + (\vec{\nabla} \varphi(x))^2 + m^2 \varphi(x)^2] + g \varphi(x)^4 \right\} d^3x, \quad (2.11)$$

which leads to the fact that $g > 0$ was in the equation to be solved, but the results were as if $g = 0$. Now, using affine quantization, it has been able to correctly solve that

equation with the presence of a new $\hbar$ -term, specifically $2\hbar^2/\varphi(x)^2$, added just after the kinetic term in the quantum Hamiltonian, which allows g to do its job correctly.

Observe that the added $\hbar$ -term was available because it required that $\varphi(x) \neq 0$. Now using standard quantum variables has lead us to

$$\mathcal{H} = \int \left\{ \frac{1}{2} [\widehat{\pi}(x)^2 + 2\hbar^2/\varphi(x)^2 + (\vec{\nabla} \varphi(x))^2 + m^2 \varphi(x)^2] + g \varphi(x)^4 \right\} d^3x. \quad (2.12)$$

It is important that Monte Carlo studies (by setting $\hbar = 1$) have confirmed the correct results of this solution because it had the $\hbar$ -term in its Hamiltonian. While canonical quantization has failed to solve this problem, affine quantization has now completely, and correctly, solved $\varphi(x)_4^4$; see [11, 16, 17].

For more than a century, we have had canonical quantization as the tool of quantization itself in which we had only Q and P along with $QP - PQ = i\hbar \mathbb{I}$ and related similar field operators which require space range from plus and minus infinity. This has forced such quantization requiring these infinite properties, but on forcefully some things need non-infinite properties to solve certain formulations.

A common example of what cannot deal with canonical quantization is the “particle in a box”, which is properly reached using some new proper quantization, that is now available under the name of affine quantization [18]. This new quantization tool can be used to solve new kinds of properties of length in the point of view in which the new procedures can use the “particle in the box” as a first example of a well-developed approach to quantization. This new procedure called affine quantization can tackle a marvelous combination of problems. This section has been chosen to tackle some examples that cannot be solved by canonical quantization, but instead requires the proper procedures leading by affine quantization. This new tool can solve the correct quantization of a grand supply of soluble problems. See for yourselves!

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Chapter 3

The Higgs Boson



*Ma perch' io non proceda troppo chiuso,
Francesco e Povertà per questi amanti
prendi oramai nel mio parlar diffuso.*

*Dante Alighieri
La Divina Commedia (canto XI paradiso)*

Abstract In this chapter, we describe the Higgs boson, the Spontaneous Symmetry Breaking mechanism for Global and Local Symmetries, and the experiment for his discovery and detection.

The *Higgs boson*, or Higgs particle, is an elementary particle in the Standard Model of particle physics. As such his waves functions are in bijective correspondence with the vectors of a finite dimensional irreducible unitary representation of its group of symmetries. In the Standard Model, the Higgs particle is a massive scalar boson with zero spin, even (positive) parity, no electric charge, and no color charge, that couples to mass. It is also very unstable, decaying into other particles almost immediately.

The Higgs wave function is a scalar field, with two neutral and two electrically charged components that form a complex doublet of the weak isospin $SU(2)$ symmetry. Its “Mexican hat-shaped” potential breaks the weak isospin symmetry of the electroweak interaction, and via the Higgs mechanism, proposed by Higgs in 1964 along with five other scientists in three teams, gives rise to some particles mass.

After a 40 year search, a subatomic particle with the expected properties was discovered in 2012 by the ATLAS and CMS experiments at the Large Hadron Collider (LHC) at CERN near Geneva, Switzerland. The new particle was subsequently confirmed to match the expected properties of a Higgs boson. Physicists from two of the three teams, Peter Higgs and François Englert, were awarded the Nobel Prize in Physics in 2013 for their theoretical predictions. Although Higgs’s name has come to be associated with this theory, several researchers between about 1960 and 1972 independently developed different parts of it.

In this chapter¹, we will work with non Euclidean field theory with real time and the field will be denoted with ϕ .

3.1 The Mathematical Observation and the Spontaneous Symmetry Breaking (SSB) Mechanism

In this section, we present the phenomenon of spontaneous symmetry breaking (SSB). According to this important and general mechanism, the symmetry of the action in Quantum Field Theory (QFT) or of the Hamiltonian in a statistical fluid is reflected on the ground state of the system.

In Sect. 3.1.1, we will show how SSB can only take place in a system with an infinite number of degrees of freedom as a field-theoretical phenomenon or in the thermodynamic limit as a statistical phenomenon. For example, it cannot occur in Quantum Mechanical (QM) systems with a finite number of variables.

We will examine the effect of SSB on different types of symmetries. In Sect. 3.1.2, we will discuss the SSB of global symmetries, and the emergence of Goldstone bosons. In Sect. 3.1.3, we will examine the SSB of local abelian symmetries which is a crucial element in the Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity, when the latter is formulated in field theoretical language [2].

3.1.1 Degenerate Vacua in QM and QFT

In this subsection, we will deal with QFT. In this case, the SSB phenomenon predicts the existence of a family of degenerate vacua that transform into each other under the action of the symmetry (global or local) group of the action instead of having a unique vacuum state which respects this symmetry. A simple example is given by Jellium [3], an electron gas, in any spatial dimension at low temperatures, in the quantum regime. Above a critical electron density, Jellium is translationally invariant. Below a critical electron density, it becomes thermodynamically favorable to develop the Wigner crystal which is a vacuum where the translational invariance is broken into a body-centered cubic lattice in 3D, a triangular lattice in 2D, and an evenly spaced lattice in 1D.

The original translation invariance of the Lagrangian is now reflected in the fact that, instead of a single vacuum state, there is a whole family of vacua related to each other by translations, since the crystallization can in principle develop in any direction. However, the system will choose one of these states as its vacuum state. The symmetry is then said to be *spontaneously broken* by the choice of a vacuum.

¹ The following Sect. 3.1 is extracted from Chap. 11 of the book “A Modern Introduction to Quantum Field Theory” by Michele Maggiore, Copyright @ Oxford University Press 2005. For details and derivations see that Ref. [1].

On the other hand, SSB is a phenomenon that cannot take place in a quantum mechanical system with a finite number of degrees of freedom. In this case, the true vacuum state is a superposition of the degenerate vacua, which respects the original symmetry. Consider, for example, the quantum mechanical problem of a particle, described by a coordinate $q(t)$, in a potential

$$V(q) = \frac{\lambda^2}{2} [q^2(t) - \eta^2]^2, \quad (3.1)$$

with λ, η parameters. This potential is shown in Fig. 3.1, and is called a double-well potential. The Lagrangian is

$$\mathcal{L} = \frac{1}{2} m \dot{q}^2 - V(q), \quad (3.2)$$

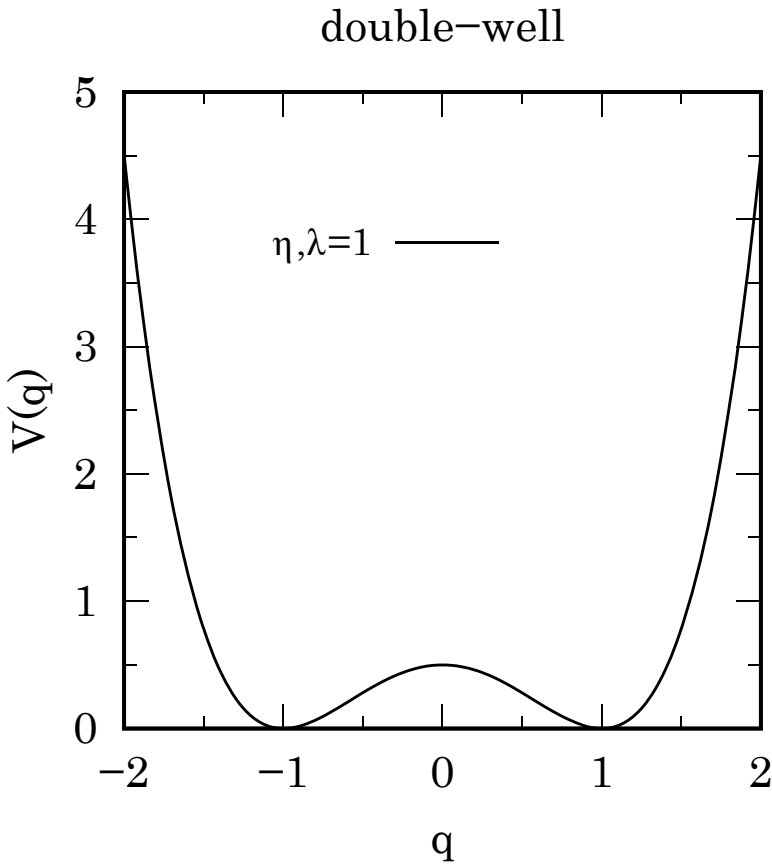


Fig. 3.1 A double-well potential of Eq. (3.1)

and is symmetric under the parity transformation $q(t) \rightarrow -q(t)$. The potential has two minima, at $q = \pm\eta$. We can solve the Schrödinger equation expanding the potential around the minimum at $q = +\eta$ in a Taylor series. If we keep only up to quadratic terms we will end up with a harmonic oscillator. We call $|+\rangle$ the ground state which will be a perturbative vacuum. We can do the same expanding around $-\eta$, and we call $|-\rangle$ the corresponding perturbative vacuum. However, the true ground state of the theory is neither $|+\rangle$ nor $|-\rangle$. At the non-perturbative level, there is a non-vanishing amplitude for the transition between these two states, due to the possibility of tunneling under the barrier which separates the two minima, and which can be computed in a semi-classical approximation. Because of the tunneling process, the Hamiltonian is not diagonal in the $|\pm\rangle$ basis. Rather, we will have $a \equiv \langle +|\mathcal{H}|+\rangle = \langle -|\mathcal{H}|-\rangle$ and $b \equiv \langle -|\mathcal{H}|+\rangle = \langle +|\mathcal{H}|-\rangle$, where $b \ll a$, since the tunneling amplitude is exponentially suppressed. Diagonalizing this Hamiltonian we immediately find that the eigenstates are the symmetric and antisymmetric combinations $|S\rangle = |+\rangle + |-\rangle$ and $|A\rangle = |+\rangle - |-\rangle$, with energies $a \pm b$, respectively. Therefore, the degeneracy between these states is lifted by the fact that $b \neq 0$, and the true ground state is the combination with energy $a - |b|$.

Under a parity transformation $q \rightarrow -q$, $|S\rangle$ is invariant, while $|A\rangle$ picks a minus sign. Recalling that physical states are defined up to an overall phase, we see that the true ground state of the Hamiltonian goes into itself under parity, and there is no SSB of the Z_2 symmetry.

Consider now a real scalar field $\phi(t, \mathbf{x})$. In natural units $\hbar = c = 1$, we denote with $\partial_\mu = \partial/\partial x^\mu$ where $x = (x^0, x^1, x^2, x^3) = (t, \mathbf{x})$, and $\mu = 0, 1, 2, 3, 4$. Consider the Lagrangian

$$\mathcal{L} = \partial^\mu \phi \partial_\mu \phi - \frac{\lambda^2}{2} [\phi^2 - \eta^2]^2. \quad (3.3)$$

Here again, we have a Z_2 symmetry $\phi \rightarrow -\phi$. The crucial difference is that the tunneling amplitude in this case is proportional to $\exp(-cV)$ with $c > 0$ a constant and V the spatial volume. This result can be understood physically by discretizing space, so that our field theory corresponds to a quantum mechanical system in which, for each spatial point $\mathbf{x}$ in volume V , we have a variable $q_{\mathbf{x}}(t) \equiv \phi(t, \mathbf{x})$, and in order to tunnel into the other vacuum each of the $q_{\mathbf{x}}$ must tunnel. Let the tunneling amplitude for a single variable $q_{\mathbf{x}}$ be proportional to $\exp(-c')$, for some constant $c' > 0$. The total amplitude is the product of the separate amplitudes so that if N is the number of lattice sites in volume V we find a tunneling amplitude proportional to $\prod_{\mathbf{x}} \exp(-c') = \exp(-c'N) = \exp(-cV)$. In an infinite volume, this amplitude vanishes and there is no mixing between the two vacua. In other words, the effective height of the barrier is infinite and therefore we truly have two distinct sectors of the theory, i.e., two different Hilbert spaces H_+ , H_- constructed above the two vacua $|\pm\rangle$. It is not possible to restore the symmetry via tunneling, and all local operators have vanishing matrix elements between a state in H_+ and a state in H_- .

A characteristic of SSB is the existence of an order parameter which takes a non-zero expectation value on the chosen vacuum. In the example of Jellium, the

order parameter is the Fourier transform of the local Density, while in the previous example, it was an element of Z_2 , $\langle\phi\rangle/\eta = \pm 1$. In the following, we will be interested in situations where the order parameter is a scalar field ϕ , real or complex. The order parameter is a quantity which is not invariant under the symmetry in question, so that a non-vanishing expectation value means that the symmetry is broken.

For a Lie group, we can restate the condition of SSB in terms of the action of the generators on the vacuum state. We denote by $U = \exp(i\theta^a T^a)$ a generic element of the symmetry group in question, and by T^a the generators. If the vacuum state is invariant, then for any value of the parameters θ^a , we have $U|0\rangle = \exp(i\alpha)|0\rangle$ for some constant phase α . In order to have SSB, we must require that $T^a|0\rangle$ is not proportional to $|0\rangle$ itself for all a .

3.1.2 SSB of Global Symmetries: Goldstone Bosons

Consider the Lagrangian for a complex scalar field

$$\mathcal{L} = \partial^\mu \phi^* \partial_\mu \phi - V(|\phi|), \quad (3.4)$$

where

$$V(|\phi|) = \frac{\lambda^2}{2} [|\phi|^2 - \eta^2]^2, \quad (3.5)$$

This Mexican-hat potential for ϕ is a double-well potential for $|\phi|$ and therefore it has a continuous set of minima. If we write $\phi = |\phi| \exp(i\alpha)$, the vacua are characterized by $\langle|\phi|\rangle = \eta$ and $\langle\alpha\rangle$ arbitrary. The Lagrangian has a *global* $U(1)$ invariance $\phi \rightarrow \exp(i\theta)\phi$ with θ an arbitrary constant. The scalar field will choose one of these vacua, so that $\langle\alpha\rangle = \alpha_0$, and the $U(1)$ symmetry is spontaneously broken. Without loss of generality, we can redefine α so that $\alpha_0 = 0$, and therefore on the vacuum $\langle\phi\rangle = \eta$. We want to understand the spectrum of the theory after SSB. This can be done studying the small oscillations around the vacuum. We therefore write

$$\phi(x) = \eta + [\chi(x) + i\psi(x)]/\sqrt{2}, \quad (3.6)$$

where χ and ψ are real fields. Observe that the set of vacua is a circle of radius η in the complex field plane, and since we are expanding around the point ($\text{Re } \phi = \eta$, $\text{Im } \phi = 0$), χ is a fluctuation in the direction orthogonal to the manifold of vacua, while ψ is a fluctuation in the tangential direction, as shown in Fig. 3.2. In other words, $\eta + i\psi$, for ψ constant and infinitesimal, is another vacuum. A small displacement in the direction of ψ does not cost energy since we are moving along a flat direction of the potential (at least to lowest order, i.e., retaining terms quadratic in ψ in the Lagrangian and neglecting cubic and higher-order terms). Instead with a small displacement in the direction of χ , we feel an approximately quadratic rise of the potential, so this

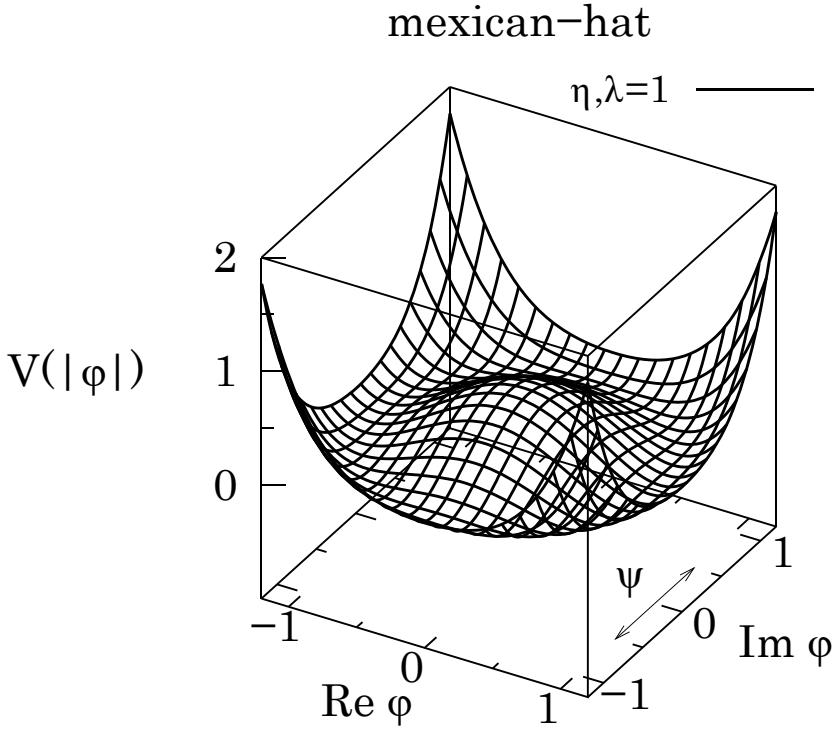


Fig. 3.2 The Mexican-hat potential of Eq. (3.5). Also shown is the direction in field space parametrized by ψ the Goldstone mode. The Higgs mode χ (not shown) is orthogonal to ψ

fluctuation costs energy. It is therefore clear that, after quantization, ψ is associated to a massless mode, while χ is a massive mode. To check this formally, we insert Eq. (3.6) into the Lagrangian (3.4), and we find

$$\mathcal{L} = \frac{1}{2} \partial^\mu \chi \partial_\mu \chi + \frac{1}{2} \partial^\mu \psi \partial_\mu \psi - \frac{\lambda^2}{8} [(2\sqrt{2}\eta)\chi + \chi^2 + \psi^2]^2, \quad (3.7)$$

We see indeed that in this Lagrangian, there is a mass term for χ , $m_\chi^2/2 = (\lambda^2/8)(2\sqrt{2}\eta)^2 = \lambda^2\eta^2$. But there is no term of the form $(1/2)m_\psi^2\psi^2$, so ψ is massless. In conclusion, in this model the $U(1)$ symmetry is spontaneously broken by the choice of the vacuum, and at the same time a massless scalar boson appears in the spectrum. This is an example of a general theorem, the Goldstone theorem, which states that, given a field theory which is Lorentz invariant, local, and has a Hilbert space with a positive definite scalar product, if a continuous *global* symmetry is spontaneously broken, then in the expansion around the symmetry-breaking vacuum

there appears a massless particle for each generator that breaks the symmetry. This particle is called a Goldstone (or Nambu–Goldstone) particle.

As in the above example, also in the general case the emergence of massless particles corresponds to the possibility of moving, in field space, in the direction of the manifold of vacua. The dimensionality of the manifold of vacua is equal to the number of generators which break the symmetry. In fact, setting the vacuum energy to zero, by definition, we have $\mathcal{H}|0\rangle = 0$. Since T^a is the generator of a symmetry transformation, it satisfies $[T^a, \mathcal{H}] = 0$ and therefore $\mathcal{H}(T^a|0\rangle) = T^a\mathcal{H}|0\rangle = 0$. So, if $T^a|0\rangle \neq 0$ (and if it is not proportional to $|0\rangle$ itself), we have found a new state with the minimum energy, i.e., another vacuum state. This is the origin of the fact that we have a Goldstone particle for each generator which breaks the symmetry.

The Goldstone theorem further states that the quantum numbers of the Goldstone particles are the same as the corresponding generator. In most cases, the global symmetry transformations are internal transformations in the field space which do not act on the Lorentz indices of the fields. For instance, in the above example, the symmetry which is broken is $U(1)$, or, equivalently, an $O(2)$ rotation symmetry in the space $(\text{Re } \phi, \text{Im } \phi)$. These rotations do not touch Lorentz indices, and therefore the generators are Lorentz scalars. Correspondingly, the associated massless particle is a spin-0 boson.

In particular, the pions are the Goldstone bosons associated to the SSB of the axial $SU(2)$ symmetry of Quantum Chromo Dynamics (QCD). They would be exactly massless if the symmetry were exact. Since it is only approximate, they are just lighter than other hadrons.

3.1.3 SSB of Local Symmetries: Abelian and Non-abelian Gauge Theories

The spontaneous breaking of a *local* symmetry, as for example, the $U(1)$ *local* transformation $\phi \rightarrow \exp[i\theta(x)]\phi$ with $\theta(x)$ the parameter of a gauge transformation, does not produce Goldstone bosons, but instead the gauge field acquires a mass proportional to the vacuum expectation value of the scalar field. This is an abelian gauge symmetry, but it is also possible to think about non-abelian gauge symmetries as, for example, the $SU(2) \times U(1)$ of the electroweak sector of the Standard Model.

In this context, the scalar field ϕ is called a *Higgs field*, and the mechanism that produces a mass for the gauge boson is called the *Higgs mechanism*. It is interesting to compare the number of degrees of freedom with and without SSB.

To understand the physical content of the theory, it is convenient to write the complex field ϕ in terms of its modulus and a phase, and to expand the modulus around η ,

$$\phi(x) = |\phi(x)|e^{i\alpha(x)} = \left[\eta + \frac{1}{\sqrt{2}}\varphi(x) \right] e^{i\alpha(x)}. \quad (3.8)$$

Now observe that we can fix the gauge freedom setting $\alpha(x) = 0$ in Eq. (3.8). In other words, we have used the gauge freedom to remove one degree of freedom from the complex field ϕ , so that we are left with just a single real scalar field φ . The phase $\alpha(x)$ parametrizes the manifold of vacua, so it is the field that, in the case of global symmetries, describes the Goldstone boson. We see that when we break a local symmetry the Goldstone boson is eliminated from the physical spectrum by gauge invariance.

If in the potential we set $\eta = 0$, then there is no SSB and the scalar field has two real components. We cannot use the gauge invariance to eliminate the phase θ as before, because when $\eta = 0$ the decomposition (3.8) of ϕ in terms of two real fields φ, θ is not well defined: in fact in this case $\varphi = \sqrt{2}|\phi|$ and therefore $\varphi \geq 0$, so it is no longer a scalar field which can freely perform at least infinitesimal fluctuations around $\varphi = 0$. Rather, gauge invariance can be used to eliminate the longitudinal components of the gauge field and the remaining gauge field has two physical degrees of freedom, the two transverse polarizations [1]. In total, we have two physical degrees of freedom from the Higgs field and two from the gauge field. After SSB, the scalar field has just one real component, but the gauge field is massive, and a massive spin-1 particle has three degrees of freedom. So again, we have $1 + 3 = 4$ degrees of freedom. So, the Higgs mechanism implies a reshuffling of the degrees of freedom.

The breaking of the symmetry takes place at the level of the vacuum. It can be shown that such a spontaneous breaking preserves a number of good properties of the unbroken theory, and in particular the theory is still renormalizable. Intuitively, this comes from the fact that at very high energies $E \gg \eta$ we can neglect η and the ultraviolet properties of the theory are the same as in the case $\eta = 0$.

This mechanism gives an effective mass to the photon in a superconductor which is the origin of the Meissner effect [2] and it gives a mass to the gauge bosons $W^\pm$ and Z^0 of the electroweak theory [4–6].

3.2 The Experiment

Proving the existence of the Higgs particle was far from easy. These are extremely difficult to produce and detect, due to the energy required to produce them and their very rare production even if the energy is sufficient. It took several decades before the first evidence of the Higgs boson could be found. Particle colliders, detectors, and computers capable of looking for Higgs bosons took roughly 40 years to develop.

The importance of this fundamental search led to the construction of one of the world's most expensive and complex experimental facilities to date, CERN's Large Hadron Collider (LHC), in an attempt to create Higgs bosons and other particles for observation and study. On 4 July 2012, the discovery of a new particle with a mass between 125 and 127 GeV/c² was announced. Physicists suspected that it was the Higgs boson. Since then, the particle has been shown to behave, interact, and decay in many of the ways predicted for Higgs particles by the Standard Model, as well as

having even parity and zero spin [7]. The latter property means that the Higgs boson is the first elementary scalar particle discovered in nature.

By March 2013, the existence of the Higgs boson was confirmed, and therefore, the concept of some type of Higgs field throughout space is strongly supported. On 14 March 2013, CERN confirmed the following:

CMS and ATLAS have compared a number of options for the spin-parity of this particle, and these all prefer no spin and even parity [two fundamental criteria of a Higgs boson consistent with the Standard Model]. This, coupled with the measured interactions of the new particle with other particles, strongly indicates that it is a Higgs boson.

The presence of the field, now confirmed by experimental investigation, explains why some fundamental particles have mass, despite the symmetries controlling their interactions imply that they should be massless. It also resolves several other long-standing puzzles, such as the reason for the extremely short distance traveled by the weak force bosons, and therefore the weak force's extremely short range.

As of 2018, in-depth research shows the particle continuing to behave in line with predictions for the Standard Model Higgs boson. More studies are needed to verify with higher precision that the discovered particle has all of the properties predicted, or whether, as described by some theories, multiple Higgs bosons exist.

The nature and properties of this field are now being investigated further, using more data collected at the LHC.

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Chapter 4

Initial Singularity Problem



*Luce et amor d'un cerchio lui comprende,
siccome questo li altri; e quel procinto
colui, che 'l cinge, solamente intende.*

*Dante Alighieri
La Divina Commedia (canto XXVII paradiso)*

Abstract In this chapter, we introduce the problem of Black Holes in Quantum Gravity and how it can be overcome with Affine Quantization.

The initial singularity problem is a long standing problem in modern cosmology. It is often believed that the effects of quantum gravity should provide an answer to this question. Renowned candidate theories for quantum gravity are loop quantum gravity and superstring theories. Loop quantum cosmology and gauge gravity duality are possible avenues of exploration [1, 2]. However other alternative or complementary approaches could be conceived. Among them, affine quantization has been recently put forward in order to quantize gravity [3–5], but has also been studied previously in [6, 7], while this approach was used to study a strong coupling limit of gravity in [8–10]. It is certainly interesting to examine the implications of this proposal. That is the use of an affine coherent state quantization program to build a correct treatment of Quantum Gravity [11]. We notice that the quantum corrections introduced in this program provide in a natural way a potential barrier term.

A detailed analysis on how affine quantization may help in formulating a valid quantum gravity action can be found in [11]. Here we just outline some of its implications.¹

¹ Much of the material in Sect. 4.1 has been extracted from our Ref. [12].

4.1 Thank the Quantum Realm for *Nothing* Ever Entering into Black Holes

While the quantum realm seems hidden, it can also reach examples of infinite energy, especially when a part of space is roughly removed until it disappears, possibly forever. Since it follows that *Nothing* can enter a region where the space is missing, the quantum realm, as seen now in affine quantization, will automatically come to help everything else by creating colossal “quantum walls” that will ensure that everything stays out of all black holes.

Here we show that the expanded quantum realm allows *Nothing* to ever fall into a black hole.

While humanity believes that the quantum realm is very weak due to a very small $\hbar$ -factor, they do not appreciate that it can be immensely strong because, effectively, selected $\hbar$ -terms can reach an infinite energy.

4.1.1 A Brief Examination of the Current Understanding of Black Holes

The current understanding of black holes is naturally from a classical viewpoint, and, to a degree, also relies on canonical quantization. In this case, it requires that the physical space exists everywhere, e.g., $-\infty < q < \infty$. Black holes have then, essentially, found that colossal quantities of trash have piled up, which are so huge that they can even develop very strong attractions of gravity.

4.1.2 A New and Very Different Analysis

4.1.2.1 A New Quantization Procedure

First of all, we introduce a new, and different, formulation of quantization procedures, which is known as **Affine Quantization**. It has the very important property that it can only exist if there are *missing parts of space*, and that is shown by incomplete regions that still remain, e.g., $0 < q$, $0 < |q|$, $|q| < b$, and especially $|q| > b > 0$, since the last example will be important for this article, and which could offer a very great distinction between this new understanding of black holes and the conventional understanding of black holes. This new quantization procedure has proven itself very well in dealing with examples that only have an **incomplete space**.

Now we will examine what could look like regions of missing space that might lead us to investigate and see if that might be black holes.

4.1.2.2 A Toy Model that Is VERY Relevant

The classical Hamiltonian for the half-harmonic oscillator is [13] $H = (p^2 + q^2)/2$, but it has been so-named because we have chosen that only $q > 0$ remains. In that case, and using affine quantization, we find that the quantum Hamiltonian is $\mathcal{H} = (P^2 + (3/4)\hbar^2/Q^2 + Q^2)/2$, with $Q > 0$. For this example, the eigenvalues are $E'_n = 2\hbar(n+1)$ for $n = 0, 1, 2, \dots$, while the eigenvalues for the well-known full-harmonic oscillator are $E_n = \hbar(n+1/2)$. Evidently, in each case, the eigenvalues are equally spaced, and the number 2 “has just played an important role”.

Since the $\hbar$ -term can become very, very, strong close to $q = 0$, it would be useful to introduce a new way of spelling the word classical, namely by **classicAL**, as a *signal* that all $\hbar$ -terms have been **included** along with the standard classical elements used for standard classical equations. Specifically, we would now like to use $H = (p^2 + (3/4)\hbar^2/q^2 + q^2)/2$, because now $q > 0$. In fact, that would help signal that its classical particles must bounce backwards at the point $q = 0$. Since each of these potential-like $\hbar$ -terms can even reach infinity, it seems only reasonable that such $\hbar$ -terms should appear together with standard polynomials in the same kind of equations. After all, you would readily accept $H = (p^2 + \gamma 10^{-50} q^{-50} + q^2)/2$ into the classical Hamiltonian family, so why not let suitable $\hbar$ -terms that *could, should, and would*, act as very useful potentials since they can reach infinity. In addition, it is also noteworthy that when affine quantization immediately finds a new missing space it **automatically** introduces a new “quantum wall” to keep everything away from that missing space.

In addition, if the remaining spatial space, $q > 0$, was partially increased, by setting it now be $(q + b) > 0$, with $b > 0$, then the new eigenvalues would still be equally spaced, and finally, when $b \rightarrow \infty$, we would correctly obtain all of the properties of its canonical quantization [14]. Effectively, all affine expressions, can eventually become a related canonical formulation just by restoring all of the missing space.

Returning to our initial expressions, observe that $q > 0$, which is our retained space, and refusing from entering our missing space, which, for this example, is $q \leq 0$, even having a classical Hamiltonian, such as $H = (p^2 + q^2)/2$, when $q \leq 0$ is no longer prohibited. It would seem to make more useful physics by adding the $\hbar$ -term that was “smart enough” to become this kind of classicAL Hamiltonian, e.g., $H = (p^2 + (3/4)\hbar^2/q^2 + q^2)/2$.

Surprisingly, our study of black holes will not be so very different than the topics of this section.

Remember that $\hbar^2$ is NOT ZERO, and that affine quantization can rigorously, and correctly, solve a very different set of problems than those of canonical quantization: specifically, affine quantization has been designed to solve ALL examples with ANY kind of missing space.

4.1.2.3 Exploiting Missing Parts of Space

We shall propose that black holes may be examined through a specific, and correct, article, namely **The Particle in a Box Warrants Examination** [15]. All that would be necessary, effectively, is to use two, very similar, Hamiltonians except that the first one is active **inside** the box, while the second one is active **outside** the box. In order to deal with the one being outside, it will be necessary to add additional potentials that can handle the complete outside space. Effectively, the second example space just has a finite section removed from the complete space. The Hamiltonians for the “particle in a box”, have been correctly created in the article just mentioned.²

It is physically correct that the $\hbar$ -terms should now also belong with the classicAL family, which has a “new spelling and meaning”, that signals that this word is now being used to **include all** $\hbar$ -terms as well, especially because all of those $\hbar$ -terms can already reach infinity, and should be allowed alongside the conventional potential terms in standard classical Hamiltonian equations. Now, both the classicAL and quantum Hamiltonians have included all $\hbar$ -terms, such as in this example, first offered in the new classicAL form:

$$H = \frac{1}{2}[p^2/m + \hbar^2(2q^2 + b^2)/(q^2 - b^2)^2 + m q^2] + V(q), \quad (4.1)$$

and second, and using the standard Schrödinger formulation, leads to

$$\mathcal{H} = \frac{1}{2}[P^2/m + \hbar^2(2q^2 + b^2)/(q^2 - b^2)^2 + m q^2] + V(q). \quad (4.2)$$

To make this example even more physical-like, we can just let $b \rightarrow b(x, t)$ in those two equations. Also, 2 or 3 spatial dimensions can be accepted, simply by changing $p \rightarrow \vec{p}$ and $q \rightarrow \vec{q}$ as well as $P \rightarrow \vec{P}$ and $Q \rightarrow \vec{Q}$.³

The authors believe that strong $\hbar$ -terms definitely belong in classicAL physics, and be included in the traditional classical equations that would be suitable, because terms, such as $2\hbar^2/q^2$, which can reach infinity, should be serving as standard potentials, and certainly such terms would deserve to be added to appropriate classicAL equations.

The authors also believe that space can be broken which leads to regions that are completely absent of any space. Of course, that would have taken huge physical efforts, but when enough trash has been closely assembled, it is very likely that it could easily destroy the local space through fantastic weight, giant explosions, and any other brutal crushing.

² The details of the $\hbar$ -terms have been taken from a special article, and while they can reach the 3/4 story extremely close to each end, the analysis in between the two ends requires special attention from page 3 in [16].

³ Although we will not need it in this article, but if the missing space is just a *single point* in space, like just removing $q = 0$, that would still require “quantum walls”, as seen in Eqs. (4.1) and (4.2), the factor b can be reduced to zero indicating that removing just a single point from space will still create “quantum walls”. That final expression could represent the birth (or death) of a black hole.

As the toy model in this Section has showed, that after suddenly removing a specific portion of space, the quantum realm will *instantly* create a “quantum wall” in order to keep everything out of the new missing space.

Now the new, and very useful, affine quantization procedures will **never** let anything fall into such a black hole. In addition, it is noteworthy that you should realize the ability to stop anything from entering a black hole because the new quantization process will keep everything out of any black hole.

You may be assured that canonical quantization may never be suitable to deal with black holes. Fortunately, this new, and very suitable, affine quantization, and its procedures, can definitely deal with incomplete space, and AQ is now available to have it be fully explained. If you wish to have a better understanding of affine quantization, you could examine a beginner’s article [17], or for more experienced people, choose article [11].

And finally, black holes are dealing with giant fires that are held surrounding the black hole itself. It is proposed now that a “quantum wall” will hold trash away from entering into the black hole, and, like any other potential would do,

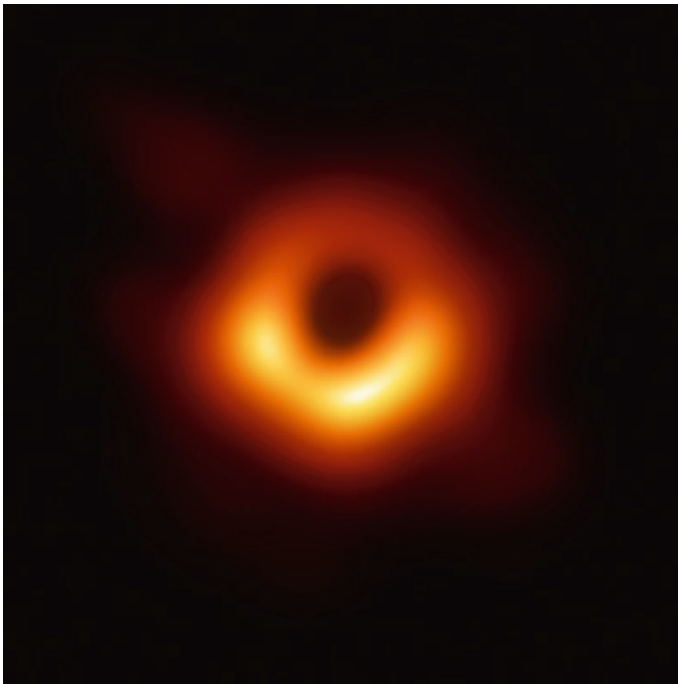


Fig. 4.1 This is the first direct image of a supermassive black hole, located at the galactic core of Messier 87 (M87*) [18, 19]. It shows 1.3 mm radio-wave emission from a heated accretion ring orbiting the object at a mean separation of 350 AU, or ten times larger than the orbit of Neptune around the Sun. The dark center is the event horizon and its shadow. The image was released in 2019 by the Event Horizon Telescope Collaboration

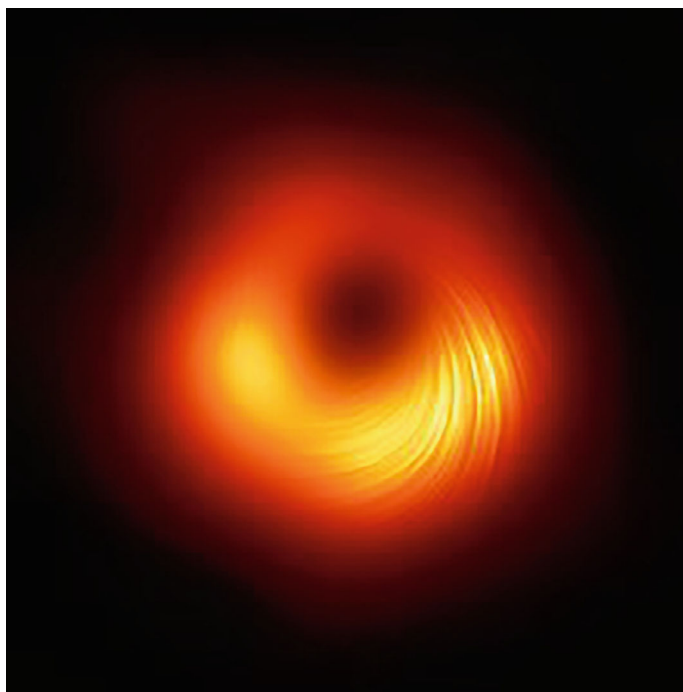


Fig. 4.2 In this image we show a view of the M87* supermassive black hole in polarized light, taken by Event Horizon Telescope and revealed on 24 March 2021. The direction of lines atop the total intensity mark the direction of the electromagnetic wave electric vector oscillations

it will glow from the burning trash, which has piled up against the “quantum wall” surrounding closely just outside of the black hole. The conventional view may not have as good an understanding of the “ring of fire” surrounding a black hole as does that of the quantum realm formulation.

The authors of this book are convinced that the standard description of black holes is very likely incorrect (see Figs. 4.1 and 4.2), and since Nature has definitely showed us how to make a “quantum wall”, the contents of this book should appear more believable than those of the standard understanding of black holes.

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Chapter 5

Quantization Procedures



*del cor de l'una de le luci nove
si mosse voce, che l'ago a la stella
parer mi fece in volgermi al suo dove;*

*Dante Alighieri
La Divina Commedia (canto XII paradiso)*

Abstract In this chapter, we review the three main quantization procedures available in Enhanced Quantization and we learn how to quantize selected problems.

Let's start by defining the Fubini-Study metric in Quantum Mechanics. Given two points $|\psi\rangle$ and $|\phi\rangle$ of the Hilbert space, the distance (length of geodesic) between them is

$$\gamma(\psi, \phi) = \arccos \sqrt{\frac{\langle\psi|\phi\rangle\langle\phi|\psi\rangle}{\langle\psi|\psi\rangle\langle\phi|\phi\rangle}}, \quad (5.1)$$

where $|\psi\rangle$ and $|\phi\rangle$ are not normalized to unit length.

The infinitesimal form of this metric may be obtained by taking $\phi = \psi + \delta\psi$ to obtain

$$\begin{aligned} \arccos \left[\frac{(\langle\psi|\psi\rangle + \langle\psi|\delta\psi\rangle)(\langle\psi|\psi\rangle + \langle\delta\psi|\psi\rangle)}{\langle\psi|\psi\rangle(\langle\psi|\psi\rangle + \langle\psi|\delta\psi\rangle + \langle\delta\psi|\psi\rangle + \langle\delta\psi|\delta\psi\rangle)} \right]^{1/2} &\approx \\ \arccos \left[1 + \frac{\langle\psi|\delta\psi\rangle\langle\delta\psi|\psi\rangle}{\langle\psi|\psi\rangle^2} - \frac{\langle\delta\psi|\delta\psi\rangle}{\langle\psi|\psi\rangle} + \dots \right]^{1/2} &\approx \\ i \left[\frac{\langle\psi|\delta\psi\rangle\langle\delta\psi|\psi\rangle}{\langle\psi|\psi\rangle^2} - \frac{\langle\delta\psi|\delta\psi\rangle}{\langle\psi|\psi\rangle} \right]^{1/2} + \dots \end{aligned}$$

So that the Fubini-Study metric will be

$$(\delta\sigma)^2 = \frac{\langle\delta\psi|\delta\psi\rangle}{\langle\psi|\psi\rangle} - \frac{\langle\psi|\delta\psi\rangle\langle\delta\psi|\psi\rangle}{\langle\psi|\psi\rangle^2}. \quad (5.2)$$

Or for a state of unit length $\langle\psi|\psi\rangle = 1$ we then find

$$(\delta\sigma)^2 = \|\delta\psi\|^2 - |\langle\psi|\delta\psi\rangle|^2, \quad (5.3)$$

where $|\dots|$ is the modulus and $\|\dots\|$ is a norm.

In the following, we will introduce three quantization procedures which define Hilbert spaces with a metric that is the one of the surface of zero curvature (the plane) through canonical quantization (CQ), the one of the surface of constant positive curvature (the sphere) through spin quantization, and the one of the surface of constant negative curvature (the pseudosphere) through affine quantization (AQ).

We could then say that these three procedures exhaust all the ones possible!¹

5.1 Canonical Quantization

Let's start with the coherent state of unit length

$$|p, q\rangle = e^{-iqP} e^{ipQ} |0\rangle, \quad (5.4)$$

where $|0\rangle$, the ground state of the Harmonic Oscillator, is the fiducial vector and $P = -i\partial/\partial q$ and $Q = q$ are the usual momentum and position operators, respectively, such that $[Q, P] = i\mathbb{I}$, where $[\dots, \dots]$ is the commutator. Moreover, $(Q + iP)|0\rangle = 0$ which implies that $\langle 0|Q|0\rangle = \langle 0|P|0\rangle = 0$. Also $e^{-ipQ} P e^{ipQ} = P + p$ by Hadamard lemma and more generally $e^{-ipQ} e^{iqP} f(P, Q) e^{-iqP} e^{ipQ} = f(P + p, Q + q)$ for a polynomial function f . So that in the classical limit $\langle p, q|f(P, Q)|p, q\rangle \rightarrow f(p, q)$, i.e., the quantum function of variables should follow the classical function of variables [3].

We find

$$\begin{aligned} \delta|p, q\rangle &= e^{-iqP} [-i\delta q P + i\delta p Q] e^{ipQ} |0\rangle \\ &= e^{-iqP} e^{ipQ} e^{-ipQ} [-i\delta q P + i\delta p Q] e^{ipQ} |0\rangle \\ &= e^{-iqP} e^{ipQ} [-i\delta q (P + p) + i\delta p Q] |0\rangle. \end{aligned} \quad (5.5)$$

¹ For a conceptually simple, geometric prescription for quantization see Refs. [1, 2].

Then

$$\begin{aligned}\langle p, q | \delta | p, q \rangle &= i \langle 0 | -\delta q (P + p) + \delta p Q | 0 \rangle = -ip\delta q, \\ |\langle p, q | \delta | p, q \rangle|^2 &= p^2(\delta q)^2.\end{aligned}\quad (5.6)$$

Also

$$\begin{aligned}\|\delta | p, q \rangle\|^2 &= \langle 0 | (-i\delta q (P + p) + i\delta p Q)^2 | 0 \rangle \\ &= \langle 0 | (\delta p Q - \delta q P)^2 + p^2(\delta q)^2 - 2p\delta q(\delta p Q - \delta q P) | 0 \rangle \\ &= \langle 0 | (\delta p Q - \delta q P)^2 + p^2(\delta q)^2 | 0 \rangle.\end{aligned}\quad (5.7)$$

So

$$\begin{aligned}(\delta\sigma)^2 &= \|\delta | p, q \rangle\|^2 - |\langle p, q | \delta | p, q \rangle|^2 \\ &= \langle 0 | (\delta p Q - \delta q P)^2 | 0 \rangle \\ &= \langle 0 | Q^2 | 0 \rangle (\delta p)^2 + \langle 0 | P^2 | 0 \rangle (\delta q)^2 - \langle 0 | QP + PQ | 0 \rangle \delta p \delta q \\ &= \langle 0 | Q^2 | 0 \rangle (\delta p)^2 + \langle 0 | P^2 | 0 \rangle (\delta q)^2 \\ &= \omega^{-1}(\delta p)^2 + \omega(\delta q)^2.\end{aligned}\quad (5.8)$$

where we used the fact that $\langle 0 | QP | 0 \rangle = \langle 0 | (PQ)^\dagger | 0 \rangle = \langle 0 | PQ | 0 \rangle^* = -\langle 0 | PQ | 0 \rangle$ and ω is a constant that does not depend on p and q .

Then we conclude that the metric of the coherent states in canonical quantization is the one of the flat (p, q) plane, i.e., the surface of “constant zero curvature”.

5.2 Spin Quantization

Let's start with the coherent state of unit length

$$|\theta, \varphi\rangle = e^{-i\varphi S_3} e^{-i\theta S_2} |s, s\rangle, \quad (5.9)$$

where $-\pi < \varphi \leq \pi$, and $-\pi/2 \leq \theta \leq \pi/2$ and $|s, s\rangle$ is the fiducial vector. The operators in this story [4] are S_i with $i = 1, 2, 3$, and which satisfy $[S_i, S_j] = i \epsilon_{ijk} S_k$, where ϵ_{ijk} is the Levi-Civita symbol in three dimensions. These operators obey $\mathbf{S}^2 = \sum_{l=1}^3 S_l^2 = s(s+1) \mathbb{I}_{2s+1}$, where $2s+1 = 1, 2, 3, \dots$ is the dimension of the spin matrices. The orthonormal eigenvectors $|s, m\rangle$ of S_3 are such that $S_3 |s, m\rangle = m |s, m\rangle$, where $m \in \{-s, -(s-1), \dots, s-1, s\}$. We can introduce $S_\pm = S_1 \pm iS_2$ so that $S_3 S_\pm |s, m\rangle = (m \pm 1) S_\pm |s, m\rangle$ and $S_+ |s, s\rangle = 0$. Also $S_1 = (S_+ + S_-)/2$ and $S_2 = (S_+ - S_-)/2i$. Therefore, $\langle s, s | S_1 | s, s \rangle = \langle s, s | S_2 | s, s \rangle = 0$. Moreover, $[S_+, S_-] = 2S_3$ so that $\langle s, s | S_1 S_2 | s, s \rangle = -\langle s, s | S_2 S_1 | s, s \rangle$. Also $e^{i\theta S_2} S_3 e^{-i\theta S_2} = S_3 \cos \theta - S_1 \sin \theta$ by Hadamard lemma.

We find

$$\begin{aligned}
 \delta|\theta, \varphi\rangle &= e^{-i\varphi S_3}[-i\delta\varphi S_3 - i\delta\theta S_2]e^{-i\theta S_2}|s, s\rangle \\
 &= e^{-i\varphi S_3}e^{-i\theta S_2}e^{i\theta S_2}[-i\delta\varphi S_3 - i\delta\theta S_2]e^{-i\theta S_2}|s, s\rangle \\
 &= e^{-i\varphi S_3}e^{-i\theta S_2}[-i\delta\varphi (S_3 \cos\theta - S_1 \sin\theta) - i\delta\theta S_2]|s, s\rangle. \quad (5.10)
 \end{aligned}$$

Then

$$\begin{aligned}
 \langle\theta, \varphi|\delta|\theta, \varphi\rangle &= \langle s, s| -i\delta\varphi (S_3 \cos\theta - S_1 \sin\theta) - i\delta\theta S_2|s, s\rangle \\
 &= -is \cos\theta \delta\varphi + i\langle s, s|S_1|s, s\rangle \sin\theta \delta\varphi - i\langle s, s|S_2|s, s\rangle \delta\theta \\
 &= -is \cos\theta \delta\varphi, \\
 |\langle\theta, \varphi|\delta|\theta, \varphi\rangle|^2 &= s^2 \cos^2\theta (\delta\varphi)^2. \quad (5.11)
 \end{aligned}$$

Also

$$\begin{aligned}
 \|\delta|\theta, \varphi\rangle\|^2 &= \langle s, s| -i\delta\varphi (S_3 \cos\theta - S_1 \sin\theta) - i\delta\theta S_2|^2|s, s\rangle \\
 &= \langle s, s|S_3^2|s, s\rangle \cos^2\theta (\delta\varphi)^2 + \langle s, s|S_1^2|s, s\rangle \sin^2\theta (\delta\varphi)^2 \\
 &\quad + \langle s, s|S_2^2|s, s\rangle (\delta\theta)^2 \\
 &= s^2 \cos^2\theta (\delta\varphi)^2 + \frac{1}{2}s \sin^2\theta (\delta\varphi)^2 + \frac{1}{2}s (\delta\theta)^2,
 \end{aligned}$$

where we used the fact that $\langle s, s|S_1^2|s, s\rangle = \langle s, s|S_2^2|s, s\rangle = s/2$.

So

$$\begin{aligned}
 (\delta\sigma)^2 &= \|\delta|\theta, \varphi\rangle\|^2 - |\langle\theta, \varphi|\delta|\theta, \varphi\rangle|^2 \\
 &= \frac{1}{2}s[(\delta\theta)^2 + \sin^2(\theta)(\delta\varphi)^2]. \quad (5.12)
 \end{aligned}$$

We can also introduce $q = \sqrt{s}\varphi$ and $p = \sqrt{s}\cos(\theta)$, with $|p, q\rangle = |p(\theta, \varphi), q(\theta, \varphi)\rangle$, which leads to

$$\begin{aligned}
 (\delta\sigma)^2 &= \|\delta|p, q\rangle\|^2 - |\langle p, q|\delta|p, q\rangle|^2 \\
 &= \frac{1}{2}[(1 - p^2/s)^{-1}(\delta p)^2 + (1 - p^2/s)(\delta q)^2]. \quad (5.13)
 \end{aligned}$$

Equation (5.12) makes it clear that we are dealing with a spherical surface with a radius of $\sqrt{s/2}$. This space is also known as a “constant positive curvature” surface.

However, Eq. (5.13) makes it clear that if $s \rightarrow \infty$, in which case both p and q span the real line, we are led to “Cartesian coordinates”, a basic property of canonical quantization.

5.3 Affine Quantization

Let's start with the coherent state of unit length

$$|p; q\rangle = e^{ipQ} e^{-i \ln(q)D} |\beta\rangle, \quad (5.14)$$

where we use the semicolon to distinguish it from the coherent state for the canonical quantization and $|\beta\rangle$ is the new fiducial vector. Q is the position operator and $D = (P^\dagger Q + Q P)/2 = D^\dagger$ the so called *dilation* operator such that $[Q, D] = iQ$ and $[Q^n, D] = inQ^n$. The affine canonical transformation consists in switching from $p \rightarrow d = pq$ and $q \rightarrow s = \ln(q)$ so that the canonical one form $p \delta q = d \delta s$.² Naturally, we must require $q > 0$ for this to make sense. Which when quantized gives the dilation operator D and the conjugated operator $S = \ln(Q)$ so that $[S, D] = [Q, P] = i$. Now $(Q - \mathbb{1} + iD)|\beta\rangle = 0$ so that $\langle\beta|Q - \mathbb{1}|\beta\rangle = \langle\beta|D|\beta\rangle = 0$ and $\langle\beta|Q|\beta\rangle = 1$. Also $e^{isD} Q e^{-isD} = e^{S+s} = Qq$ by Hadamard lemma.

We find

$$\begin{aligned} \delta|p; q\rangle &= e^{ipQ} \left[i \delta p Q - i \frac{\delta q}{q} D \right] e^{-i \ln(q)D} |\beta\rangle \\ &= e^{ipQ} e^{-i \ln(q)D} e^{i \ln(q)D} \left[i \delta p Q - i \frac{\delta q}{q} D \right] e^{-i \ln(q)D} |\beta\rangle \\ &= e^{ipQ} e^{-i \ln(q)D} \left[i \delta p Qq - i \frac{\delta q}{q} D \right] |\beta\rangle. \end{aligned} \quad (5.15)$$

Then

$$\begin{aligned} \langle p; q | \delta | p; q \rangle &= iq \delta p, \\ |\langle p; q | \delta | p; q \rangle|^2 &= q^2 (\delta p)^2. \end{aligned} \quad (5.16)$$

² Consider $A \times B = C$, as well as $A = B/C$. If $B = C = 0$, what is A ? If $B = C = \infty$, what is A ? To ensure getting A one must require $0 < |B| \text{ \& } |C| < \infty$. This is good mathematics, but physics has an opinion as well. Consider $mv = p$. If the velocity $v = 0$, then the momentum $p = 0$, which makes good sense. However, if the mass $m = 0$ and the velocity $v = 9$, then the momentum, $p = 0$, makes bad physics. However, if any of them are infinite, that is certainly bad math as well as bad physics.

We will especially use this topic for the dilation variable $d = pq$, where q is the coordinate of a position and p denotes its time derivative (times its mass too). The position $q(t)$ is continuous, while $p(t)$ is traditionally continuous, but it can change sign, like bouncing a ball off a wall.

Also

$$\begin{aligned}
 \|\delta|p; q\rangle\|^2 &= \langle\beta| \left| i \delta p Q q - i \frac{\delta q}{q} D \right|^2 |\beta\rangle \\
 &= \langle\beta| q^2 (\delta p)^2 Q^2 + \frac{(\delta q)^2}{q^2} D^2 - \delta p \delta q (QD + DQ) |\beta\rangle \\
 &= \langle\beta| Q^2 |\beta\rangle q^2 (\delta p)^2 + \langle\beta| D^2 |\beta\rangle \frac{(\delta q)^2}{q^2}, \tag{5.17}
 \end{aligned}$$

where we used the fact that $\langle\beta| QD |\beta\rangle = \langle\beta| (DQ)^\dagger |\beta\rangle = \langle\beta| DQ |\beta\rangle^* = -\langle\beta| DQ |\beta\rangle$.

So

$$\begin{aligned}
 (\delta\sigma)^2 &= \|\delta|p; q\rangle\|^2 - |\langle p; q | \delta|p; q\rangle|^2 \\
 &= \langle\beta| (Q - \mathbb{1})^2 |\beta\rangle q^2 (\delta p)^2 + \langle\beta| D^2 |\beta\rangle \frac{(\delta q)^2}{q^2} \\
 &= \beta^{-1} q^2 (\delta p)^2 + \beta \frac{(\delta q)^2}{q^2}, \tag{5.18}
 \end{aligned}$$

where $\langle\beta| (Q - \mathbb{1})^2 |\beta\rangle = \langle\beta| Q^2 - \mathbb{1} + 2Q |\beta\rangle = \langle\beta| Q^2 - \mathbb{1} |\beta\rangle$.

Then we conclude that the metric of the coherent states in affine quantization is the one of the surface (p, q) of “constant negative curvature” of magnitude $-2/\beta^3$, i.e., the pseudosphere. Accidentally I already met this very interesting Riemannian surface during my studies in statistical physics [5].

We can even change $q \rightarrow q + b$ so that $s = \ln(q) \rightarrow \ln(q + b)$ which now make sense only for $q + b > 0$. This changes the Fubini-Study metric to

$$(\delta\sigma)^2 = \beta^{-1} (q + b)^2 (\delta p)^2 + \beta \frac{(\delta q)^2}{(q + b)^2}. \tag{5.19}$$

If we now choose $b \rightarrow \infty$ and at the same time let $\beta \rightarrow \beta + \omega b^2$ we get

$$(\delta\sigma)^2 = \omega^{-1} (\delta p)^2 + \omega (\delta q)^2, \tag{5.20}$$

now with $q \in \mathbb{R}$, which, once again, applies to canonical quantization. Briefly stated, we can arrange that $AQ \rightarrow CQ$!

³ Note that while constant zero and positive curvatures can be seen in our three spatial dimensions, a visualization of a complete constant negative curvature is not possible. A glance of one would be a single point on a saddle, namely the highest point from the rider's feet direction, and the lowest point from the horse's head direction.

Summarizing Constant Curvatures and Coherent States

These three stories complete our family of “constant curvature” spaces, specifically, constant positive, zero, and negative curvatures. Additionally, the various coherent states can be used to build “bridges” in each case that enable one to jump from the classical realm to the quantum realm or jump in the other direction whenever that is feasible.

5.4 Learning to Quantize Selected Problems

We begin⁴ with two different quantization procedures, and two simple, but distinct, problems one of which is successful and the other one is a failure in trying to use both of the quantization procedures on each example.

This exercise serves as a prelude to a valid and straightforward clarification of the fact that affine quantization and canonical quantization solve completely different sets of problems. This fact will help us when we turn to the quantization of field theories (and of gravity) in later chapters.

5.4.1 Choosing a Canonical Quantization

The classical variables, p & q , that are elements of a constant zero curvature, better known as Cartesian variables, such as those featured by Dirac [6], are promoted to self-adjoint quantum operators $P (= P^\dagger)$ and $Q (= Q^\dagger)$, ranged so that $-\infty < P \text{ \& } Q < \infty$, and scaled so that $[Q, P] = i\hbar \mathbb{I}$.⁵

5.4.1.1 First Canonical Example

Our example is just the familiar harmonic oscillator, for which $-\infty < p \text{ \& } q < \infty$ and a Poisson bracket $\{q, p\} = 1$, also a classical Hamiltonian, with the common factors $m = \omega = 1$, given by $H(p, q) = (p^2 + q^2)/2$. The quantum Hamiltonian is $\mathcal{H}(P, Q) = (P^2 + Q^2)/2$, and Schrödinger’s representation is given by $P =$

⁴ Parts of this Section are reproduced from the article [4] “The Magnificent Realm of Affine Quantization: valid results for particles, fields, and gravity” by J. R. Klauder and R. Fantoni, published in Axioms, 2023, under the terms of the Creative Commons Attribution License (CC BY 4.0).

⁵ In particular, in [6], the mid-page of 114, Dirac wrote “However, if the system does have a classical analogue, its connexion with classical mechanics is specially close and one can usually assume that the Hamiltonian is the same function of the canonical coordinates and momenta in the quantum theory as in the classical theory † Footnote †: This assumption is found in practice to be successful only when applied with the dynamical coordinates and momenta referring to a Cartesian system of axes and not to more general curvilinear coordinates.”

$-i\hbar(\partial/\partial x)$ and $Q = x$, for $-\infty < x < \infty$. Finally, for our example, Schrödinger's equation is given by

$$i\hbar(\partial\psi(x, t)/\partial t) = (-\hbar^2\partial^2/\partial x^2 + x^2)/2 \psi(x, t) . \quad (5.21)$$

Solutions to Eq. (5.21) for our example are well known. In particular, for the harmonic oscillator, the eigenvalues are given by $E_n = \hbar(n + 1/2)$ for $n = 0, 1, 2, \dots$, and the eigenfunctions (with $\hbar = 1$) are given by $\psi_n(x) = N_n H_n(x) e^{-x^2/2}$ with $n = 0, 1, 2, \dots$. Here, N_n serves to enforce normalization, and the remainder is

$$H_n(x) e^{-x^2/2} = e^{x^2/2} (-d/dx)^n e^{-x^2} . \quad (5.22)$$

This model is one of the most well understood of all examples.

5.4.1.2 Second Canonical Example

For our next example we keep the same classical Hamiltonian, and we retain $-\infty < p < \infty$, but now we restrict $0 < q < \infty$. This new model is called the “half-harmonic oscillator”. It follows that the operator $P^\dagger \neq P$, which leads to a different behavior to that when P is self adjoint, i.e., $P^\dagger = P$. In particular, this can lead to infinitely many different self-adjoint Hamiltonians each of which passes to the same classical Hamiltonian that would be $(p^2 + q^2)/2$ in this case. Just two of the different quantum Hamiltonians could be $\mathcal{H}_0(P, Q) = (PP^\dagger + Q^2)/2$, while the other is $\mathcal{H}_1(P, Q) = (P^\dagger P + Q^2)/2$. Clearly, both of these quantum Hamiltonians lead to the same classical Hamiltonian, namely $(p^2 + q^2)/2$, when $\hbar \rightarrow 0$.⁶

This judgement renders the canonical quantization of the half-harmonic oscillator to be an invalid quantization.

5.4.1.3 First Affine Example

The traditional classical affine variables are $d \equiv pq$ and $q > 0$, and they have a Poisson bracket given by $\{q, d\} = q$. In addition, we can choose a different dilation variable, $d = p(q + b)$, for which $-b < q < \infty$, generally, with $b > 0$. For very large b we can approximate a full-line harmonic oscillator and even see what happens if we choose $b \rightarrow \infty$ to mimic the full-line story.

The classical affine variables now are $-\infty < d \equiv p(q + b) < \infty$ and $0 < (q + b) < \infty$, while the classical harmonic oscillator Hamiltonian is given by $H'(d, q) = [d^2/(q + b)^2 + q^2]/2$, an expression that obeys $H(p, q) = (p^2 + q^2)/2$ albeit that $-b < q < \infty$.

⁶ Here is one example of infinitely many quantum Hamiltonians for the half-harmonic oscillator, when $P^\dagger \neq P$, would be $[(P^\dagger)^{n+4}/P^{n+2} + P^{n+4}/P^{\dagger n+2}]/2 + Q^2/2$, for all $n = 0, 1, 2, \dots$.

Now we consider basic quantum operators, namely $D = [P^\dagger(Q + b) + (Q + b)P]/2$ and $Q + b$, which lead to $[Q + b, D] = i\hbar(Q + b)$, along with $Q + b > 0$. The quantum “partial-harmonic oscillator” is now given by

$$H'(D, Q) = [D(Q + b)^{-2}D + Q^2]/2 = [P^2 + (3/4)\hbar^2/(Q + b)^2 + Q^2]/2, \quad (5.23)$$

while, in a proper limit, an affine quantization *becomes* a canonical quantization when the partial real line ($-b < q$ & $Q < \infty$) is stretched to its full length, ($-\infty < q$ & $Q < \infty$).

Evidently, an affine quantization fails to quantize a full-harmonic oscillator.

5.4.1.4 Second Affine Example

The common canonical operator expression, $[Q, P] = i\hbar\mathbb{I}$, directly implies $[Q, (P^\dagger Q + QP)/2] = i\hbar Q$, which are the basic affine operators.

To confirm this affine expression, let us multiply $i\hbar\mathbb{I} = [Q, P]$ by Q , which gives $i\hbar Q = (Q^2 P - Q P Q + Q P Q - P Q^2)/2$, i.e., $i\hbar Q = [Q, (QP + PQ)/2]$, which is the basic affine expression, $[Q, D] = i\hbar Q$, where $D \equiv (PQ + QP)/2 \equiv (P^\dagger Q + QP)/2$. This derivation assumes that $Q > 0$ or $Q < 0$. Canonical quantization implies affine quantization, but adds a limitation, for classical as well as quantum, on the coordinates.

Regarding our problem, now with $b = 0$, and so the classical affine variables are $d \equiv pq$ and $q > 0$, which lead to the half-harmonic oscillator $H'(d, q) = (d^2/q^2 + q^2)/2$. The basic affine quantum operators are D and Q , where $D (= D^\dagger)$ and $Q > 0 (= Q^\dagger > 0)$. These quantum variables lead to $[Q, D] = i\hbar Q$. The half-harmonic oscillator quantum Hamiltonian is given by $\mathcal{H}'(D, Q) = (DQ^{-2}D + Q^2)/2$, and Schrödinger's representation is given by $Q \rightarrow x > 0$ and

$$D = -i\hbar[x(\partial/\partial x) + (\partial/\partial x)x]/2 = -i\hbar[x(\partial/\partial x) + 1/2]. \quad (5.24)$$

Finally, Schrödinger equation is given by

$$\begin{aligned} i\hbar(\partial\psi(x, t)/\partial t) &= \\ &= [-\hbar^2(x(\partial/\partial x) + 1/2)x^{-2}(x(\partial/\partial x) + 1/2) + x^2]/2 \psi(x, t) \\ &= [-\hbar^2(\partial^2/\partial x^2) + (3/4)\hbar^2/x^2 + x^2]/2 \psi(x, t). \end{aligned} \quad (5.25)$$

We note that kinetic factors, such as P and D , can annihilate separate features. Adopting Schrödinger's representation, it follows that $P1 = 0$ while $Dx^{-1/2} = 0$. We will exploit this simple fact in later chapters.

Solutions of (5.25) have been provided by Gouba [7]. Her solutions for the half-harmonic oscillator contain eigenvalues that are equally spaced as are the eigenvalues of the full-harmonic oscillator, although the spacing itself differs in the two cases. The

relevant differential equation in (5.25) is known as a “spiked harmonic oscillator”, and its solutions are based on confluent hypergeometric functions. It is noteworthy that every eigenfunction, $\psi_n(x) \propto x^{3/2}(\text{polynomial}_n)e^{-x^2/2\hbar}$, which applies for all $n = 0, 1, 2, \dots$. The leading factor of the eigenfunctions, i.e., $x^{3/2}$, provides a continuous result after the first derivative, but the second derivative could lead to an $x^{-1/2}$ behavior, except that $[-d^2/dx^2 + (3/4)/x^2] x^{3/2} = 0$. This zero ensures that after two derivatives, the wave function is still finite, continuous, and belongs in a Hilbert space.⁷

It is interesting to consider an increase in the coordinate space by choosing $x + b > 0$. This leads to a related Schrödinger equation, given by

$$[-\hbar^2 (\partial^2/\partial x^2) + (3/4)\hbar^2/(x+b)^2 + x^2]/2 \psi(x, t) = E_b \psi(x), \quad (5.26)$$

which has been shown to also have equally spaced eigenvalues that become narrower as b becomes larger. Moreover, if $b \rightarrow \infty$, then the $\hbar$ -term disappears and the full-harmonic oscillator, with its canonical quantization features, is fully recovered [8]. In this fashion, we observe that AQ can pass to CQ, but the reverse is, apparently, impossible.

Finally, we can assert that an affine quantization of the half-harmonic oscillator can be considered to be a correctly solved problem.

5.4.1.5 A Canonical Version of the Half-Harmonic Oscillator

We start again with the classical Hamiltonian for the half-harmonic oscillator which is still $H = (p^2 + q^2)/2$ and $q > 0$, but this time we will use different coordinates. To let our new coordinate variables span the whole real line, which makes them “Ashtekar-like” [9–11], we choose $q = s^2$, where $-\infty < s < \infty$. Thus, s is the new coordinate. For the new momentum, r , we choose $p = r/2s$. We choose it because the Poisson bracket $\{s, r\} = \{\sqrt{q}, 2p\sqrt{q}\} = 1$.⁸ The classical Hamiltonian now becomes $H = (p^2 + q^2)/2 = (r^2/4s^2 + s^4)/2$.

5.4.1.6 A CQ Attempt to Solve the Half-Harmonic Oscillator

For quantization, the new variables use canonical quantum operators, $r \rightarrow R$ and $s \rightarrow S$, with $[S, R] = i\hbar\mathbb{I}$. Following the CQ rules, this leads to $\mathcal{H}_{CQ} = [R S^{-2} R/4 + S^4]/2 \leq \infty$. This quantum operator, using canonical operators where

⁷ There are examples in which a/x^2 , with $a > 0$, such potentials are studied, but some are negative, i.e., $-a/x^2$, with $a > 0$, which has a completely different behavior.

⁸ It may be noticed that while $q > 0$, and now $q = s^2$, this would imply that $s \neq 0$. However, we will skip over this “unimportant point” until later.

$[S, R] = i\hbar\mathbb{I}$, is quite different from the affine expression $\mathcal{H}_{AQ} = [DQ^{-2}D + Q^2]/2 < \infty$, rearranged into canonical operators with $[Q, P] = i\hbar\mathbb{I}$, that leads to $\mathcal{H}_{AQ} = [P^2 + (3/4)\hbar^2/Q^2 + Q^2]/2 < \infty$.

It is self-evident that these two canonical quantum Hamiltonian operators, $\mathcal{H}_{AQ}$ and $\mathcal{H}_{CQ}$, have different eigenfunctions and eigenvalues. Does it matter that $\mathcal{H}_{AQ} < \infty$ while $\mathcal{H}_{CQ} \leq \infty$, due to $S = 0$ while $R \neq 0$? It is clear that answers to these questions are “No”. Trying to quantize the half-harmonic oscillator, using CQ variables, has led to physically incorrect results.

Now we examine a very different model using both CQ and AQ.

5.5 Using CQ and AQ to Examine “The Particle in a Box” [4]

The quantum mechanics problem of a particle in a box as found in textbooks is lacking of mathematical rigor as we will show in this section.⁹

5.5.1 An Example that Needs More Analysis

This model has often been used in teaching and it is introduced early in the process as an easy example to solve. The classical Hamiltonian for this model is simply $H = p^2$, allowing, for simplicity, that $2m = 1$. Now the coordinate space is $-b < q < b$, where $0 < b < \infty$ (which also may be chosen as $0 < q < 2b \equiv L < \infty$). To accommodate the CQ operators, we assume that outside the box there are infinite potentials that force any wave functions to be zero in the entire outside region where $|x| \geq b$. Inside the box we have the quantum equation

$$-\hbar^2(d^2\phi_n(x)/dx^2) = E_n\phi_n(x) . \quad (5.27)$$

Evidently, cos and sin are relevant. In particular, $\phi(-b) = \phi(b) = 0$ is necessary to continuously join the squashed wave functions, $\phi(|x| \geq b) = 0$. This leads to eigenfunctions which are $\cos(n\pi x/2b)$ for $n = 1, 3, 5, \dots$ and $\sin(n\pi x/2b)$ for $n = 2, 4, 6, \dots$. That leads to the eigenvalues $n^2\pi^2/4b^2$, now for $n = 1, 2, 3, 4, \dots$

⁹ Parts of this Section are reproduced from the article “The Magnificent Realm of Affine Quantization: valid results for particles, fields, and gravity” by J. R. Klauder and R. Fantoni, published in Axioms, 2023, under the terms of the Creative Commons Attribution License (CC BY 4.0).

5.5.1.1 Failure of the Canonical Quantization of the Particle in a Box

While the statements in the last section seem to be correct, there is a problem. Let us focus on the ground state, $\cos(\pi x/2b)$. We need to consider two derivatives of this function, so let us start with $\cos'(\pi x/2b) = -(\pi/2b) \sin(\pi x/2b)$ which leads to $\cos'(\pm\pi/2) = \mp\pi/2b$, i.e., the first derivative is *not* a continuous function with the squashed portion. This forces the second derivative to contain two factors proportional to $\delta(|x| = b)$, the Dirac delta function $\delta(x)$, which vanishes everywhere but $x = 0$ where $\delta(0) = \infty$, such that $\int_{-a}^{a(>0)} \delta(x) dx = 1$. It now follows that $\int \delta(x)^2 dx = \infty$, which then excludes such a function, which is supposed to be finite, e.g., $\int |\phi(x)|^2 dx < \infty$, to join any Hilbert space.

In summary, we conclude that by using CQ, the standard treatment and results for the particle in a box are incorrect.

The reduced coordinate space now requires a newly named dilation variable, $d' = p(b+q)(b-q) = p(b^2 - q^2)$, along with accepting only $-b < q < b$. Using affine variables, the classical Hamiltonian now becomes $H' = d'^2/(b^2 - q^2)^2$. Following the affine quantization rules, means that the $D' = [P^\dagger(b^2 - Q^2) + (b^2 - Q^2)P]/2$, and the quantum Hamiltonian is

$$\mathcal{H}' = D'(b^2 - Q^2)^{-2}D' = P^2 + \hbar^2[2Q^2 + b^2]/[b^2 - Q^2]^2. \quad (5.28)$$

The new $\hbar$ -expression is unraveled later in Sect. 6.3.2.

When comparing the different $\hbar$ -terms, we find, with using $Q \rightarrow x$, that if $x \simeq \pm b$, then $[2x^2 + b^2]/(b^2 - x^2)^2 \simeq 3b^2/(b \mp x)^2 4b^2$, which mimics the (3/4)-factor for the half-harmonic oscillator. This implies that the x term in eigenfunctions, extremely close to either $\pm b$, should be like $\psi(x) \simeq (b^2 - x^2)^{3/2}$ (*remainder*).

A very different use of (5.28) is to *accept* the outside space, $|x| > b$, and *reject* $|x| < b$, which then becomes an “anti-box”.

Note that this system has a similarity to a toy “black hole”. It could happen that particles would pile up close to an “end of space”, while having been attracted there by a simple, “gravity-like”, pull of a potential, such as $V(x) = W^2 x^4$. If you choose AQ, then the barracked, $\hbar$ -like term, in (5.28), would prevent the particles from falling “out of space”, while the shores exhibit light from the fires of trapped trash.

5.5.1.2 Removing a Single Point

Assuming that we still have chosen the outside, $|x| > b$, coordinates, it is noteworthy that if we focus on the region where $b \rightarrow 0$, while insisting that $|x| > 0$. In this case, the $\hbar$ -term becomes $2\hbar^2/x^2$. However, the previous eigenfunction behavior of $(x^2 - b^2)^{3/2}$, now with $x^2 > b^2$, implies that any eigenstates (again, having potentials, like $V(x) = |x|^r$, for $r \geq 2$, that reach infinity) must start like $\psi_n(x) \simeq x^3$ (*remainder_n*). This offers effective continuity for the eigenfunction and its first two derivatives, even though $x \neq 0$ can permit a more different behavior on either side of $x = 0$. This,

then, is the “cost” to remove a single point in the usual coordinate space, e.g., in this case, removing just the single point at $q = 0$.

This result has been made possible using AQ and not using CQ, which requires including all x , i.e., $-\infty < x < \infty$.

A Vector Version: The point we now wish to remove is $\vec{q} = 0$; stated, we want to retain all the variables that obey $\vec{q}^2 > 0$ and all those of $\vec{p}^2 \geq 0$. In addition, we introduce $\vec{P}^2 = \sum_{j=1}^s P_j^2$ and $\vec{Q}^2 = \sum_{j=1}^s Q_j^2 > 0$.

Using these variables, we are led to $d^* = |\vec{p}|(\vec{q}^2 - b^2)$, which leads to $\vec{p}^2 = d^{*2}/(\vec{q}^2 - b^2)^2$. Quantizing, we have $D^* = [|\vec{P}|(\vec{Q}^2 - b^2) + (\vec{Q}^2 - b^2)|\vec{P}|]/2 (= D^{*\dagger})$. Adopting the kinetic factor, $D^*(\vec{Q}^2 - b^2)^{-2}D^*$, that equation also unfolds, in a fashion similar to that shown in Sect. 6.3.2, below, and leads to the quantum Hamiltonian

$$\mathcal{H} = \frac{1}{2} [\vec{P}^2 + \hbar^2(2\vec{Q}^2 + b^2)/(\vec{Q}^2 - b^2)^2] + V(\vec{Q}^2). \quad (5.29)$$

Just by sending $b^2 \rightarrow 0$, we achieve the situation where only the single point, i.e., $\vec{q}^2 = 0 \rightarrow \vec{Q}^2 = 0$ is removed from our s -dimensional space. The quantum Hamiltonian in this case is

$$\mathcal{H}_s = \frac{1}{2} [\vec{P}^2 + 2\hbar^2/\vec{Q}^2] + V(\vec{Q}^2). \quad (5.30)$$

To offer a justification that this relation holds for all $\vec{Q}$ including just the case where $s = 1$, i.e., just Q^2 . To do so, let us introduce the wave function $\psi(x) = U(x) W_B(Bx_j)$, by introducing a partial expectation of the Hamiltonian given by

$$\begin{aligned} & \int W_B(Bx_j)^* [\vec{P}^2 - 2V(x^2)] W_B(Bx_j) d^{s-1}x \\ &= \int W_B(Bx_j)^* 2\hbar^2[2/(x^2 + \sum_{j=2}^s x_j^2)] W_B(Bx_j) d^{s-1}x \end{aligned} \quad (5.31)$$

in which we have integrated all x_j except $x = x_1$. Now, for all, but x_1 , we let $x_j \rightarrow x_j/B$, which changes the previous equation to become

$$\begin{aligned} & \int W_C(x_j)^* [\vec{P}^2 - 2V(x^2 + B^{-2}\sum_j x_j^2)] W_C(x_j) d^{s-1}x \\ &= \int W_C(x_j)^* 2\hbar^2[2/(x^2 + B^{-2}\sum_j x_j^2)] W_C(x_j) d^{s-1}x. \end{aligned} \quad (5.32)$$

The purpose of this exercise is to show that the original quantum Hamiltonian (5.30) for s many dimensions holds the equation for a final quantum Hamiltonian (5.32) as $B \rightarrow \infty$ for a single dimension.

Briefly stated, an $(s - 1)$ -dimensional reduction may be arranged that can force all of those coordinates to become zero. This leaves behind just one of the coordinates, which is part of a proper equation, and is already waiting to fulfill its duty.¹⁰

5.5.2 *Lessons from Canonical and Affine Quantization Procedures*

An important lesson from the foregoing set of examples is that canonical quantization requires special classical variables, i.e., $-\infty < p \text{ \& } q < \infty$, that create a flat surface, to be promoted to valid quantum operators that satisfy $-\infty < P \text{ \& } Q < \infty$. However, an affine quantization requires different classical variables, e.g., $-\infty < d_b = p(b + q) < \infty$ and $-b < q < \infty$, chosen so that $0 < b < \infty$, to be promoted to valid affine quantum operators, which satisfy $-\infty < D < \infty$ and $-b < Q < \infty$, provided that the classical variables arise from a constant negative curvature.

The essential information from this exercise is that affine quantization variables are created from canonical quantization variables and they permit—classical and quantum alike—in having a limited behavior where $-b < q \text{ \& } Q < \infty$, b is finite, and $-\infty < d \text{ \& } D < \infty$.

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¹⁰ Additional x_j factors may be made active by simply removing their B factor from the beginning.

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Chapter 6

Real Scalar Field Theory



*Tu se' omai al purgatorio giunto:
vedi là il balzo che'l chiude dintorno;
vedi l'entrata là've par digiunto.*

*Dante Alighieri
La Divina Commedia (canto IX purgatorio)*

Abstract In this chapter, we present the quantum relativistic Euclidean real scalar field theories of interest as treated through Canonical and Affine Quantizations, the Scaling Regularization necessary in Affine Quantization is discussed, and the applications to a restricted field space are treated.

In this chapter,¹ we present the *real* scalar field theories φ_n^r (covariant and ultralocal) studied in our collaboration. The simulations of these theories on a lattice through the Path Integral Monte Carlo (PIMC) method will be presented in the next Chap. 7 in a unified way. In particular, we present our results for the covariant $r = 12, n = 3$ and $r = 4, n = 4$. For the ultralocal $r = 4, n = 2$, we refer the reader to our Ref. [3].

In Chap. 8, we apply PIMC to a particular *complex* scalar field in order to study the Higgs Mexican-hat case (see Chap. 3 and Fig. 3.2) as a standalone presentation.

6.1 Introduction

Consider a real² scalar field $\varphi(x)$ where x are the spacetime coordinates. The family of covariant relativistic scalar field theories we consider, $(\varphi^r)_n$, have classical Hamiltonians given by

¹ Much of the material in this chapter has been extracted from our Refs. [1, 2].

² We only studied a complex scalar field in Ref. [4] that will be discussed in Chap. 8.

$$H[\pi, \varphi] = \int \left\{ \frac{1}{2} [\pi(x)^2 + (\nabla\varphi(x))^2 + m^2 \varphi(x)^2] + g \varphi(x)^r \right\} d^s x, \quad (6.1)$$

where the bare mass $m > 0$, the bare coupling constant $g \geq 0$, r , an even integer, is the power of the interaction term,³ and s is the number of spatial dimensions. As classical elements they lead to suitable equations of motion and these solutions automatically guarantee that, for $\beta > 0$, all such solutions obey the rule that $\int_0^\beta dt \int H[\pi(x, t), \varphi(x, t)] d^s x < \infty$.

However, acceptable classical solutions do not tell the whole story. The domain of the example in (6.1) includes the complete set of *arbitrary continuous paths*, $\pi(x, t)$ and $\varphi(x, t)$, that determine the domain

$$\mathcal{D}[\pi, \varphi] = \left\{ \pi, \varphi \left| \int_0^\beta dt \int H[\pi(x, t), \varphi(x, t)] d^s x < \infty \right. \right\}. \quad (6.2)$$

This expression for the domain is unchanged if the interaction term is excluded, while, on the other hand, the given domain will be dramatically reduced from the true “free theory” domain if the interaction term is sufficiently strong and has been introduced. These questions can be answered if we show the domains may be studied.

6.1.1 Review of Principal Domains

The term $\pi(x, t)^2$ is equal to $\dot{\varphi}(x, t)^2$, and if we include t as just another spatial variable the classical Hamiltonian becomes

$$H[\varphi] = \int \left\{ \frac{1}{2} [(\nabla\varphi(x))^2 + m^2 \varphi(x)^2] + g \varphi(x)^r \right\} d^n x, \quad (6.3)$$

where now $x = (x_0, x_1, x_2, \dots, x_s)$, where $x_0 = ct$ and $n = s + 1$ with c the speed of light constant. The contribution of the separate terms can be captured if we observe that the three following cases must be treated separately and constitute unitarily inequivalent quantizations:

$$\left[\int \varphi(x)^r d^n x \right]^{2/r} < \text{or} = \text{or} > \int [(\nabla\varphi(x))^2 + m^2 \varphi(x)^2] d^n x. \quad (6.4)$$

The domain of this expression consists of all $\{\varphi(x)\}$ for which $H[\varphi] < \infty$. For a given finite spacetime dimension n and power r , it is of considerable interest to learn if the domain changes when the interaction coupling constant changes from $g = 0$ to $g > 0$. The study of that issue for all $\{\varphi(x)\}$ involves an explicit expression

³ Note that the self-interaction term $V(\varphi) = \frac{1}{2}m^2\varphi^2 + g\varphi^r$ is just a single well with minimum at the origin $\varphi = 0$ for real masses but becomes a double well with minima at $\varphi = \pm\Phi$ with $\Phi = (gr/m^2)^{1/(2-r)}$, for complex masses.

in which t becomes an additional “spatial variable”

$$\left[\int \varphi(x)^r d^n x \right]^{2/r} = C \int [(\nabla \varphi(x))^2 + m^2 \varphi(x)^2] d^n x . \quad (6.5)$$

If C is bounded above for all φ , then the domain of H is the same with $g = 0$ or $g > 0$. If $C = \infty$, then the domain of H is larger when $g = 0$ than it is when $g > 0$. It follows [5, 6] that the domain does not change provided that $r < 2n/(n - 2)$. If, on the other hand, $r > 2n/(n - 2)$, then the domain of H drops as soon as $g > 0$, and thus when one seeks the domain in the limit that $g \rightarrow 0$, continuity forces the resultant domain to be the smaller domain. In other words, the domain where the CQ action is finite $\mathcal{D}_{g>0} \subset \mathcal{D}_{g=0}$ and the domains change because of reducing g back to zero will only retain the smaller version of the domain by continuity, and that will not be the theory you started out with so that the CQ model is trivial.

The focus hereafter, in this section, is on the case $r = 2n/(n - 2)$, and more explicitly, we choose $r = n = 4$.⁴ This model has been studied by applying canonical quantization, and the universally accepted result [7–9] is that this model becomes a “free model” despite the presence of the interaction and $g > 0$. Such a result may be considered as a quantum failure.

Additional efforts has been made in Refs. [10, 11] to quantize $(\varphi^4)_4$ models using alternative procedures that, regrettably, have also led only to a “free theory”.

Affine quantization can account for certain classical models that experience two different classical domains, one (“free”) without an interaction term, $g = 0$, and one (“non-free”) with the interaction term, $g > 0$. If necessary, such models automatically choose the smaller domain as $g \rightarrow 0$ by simple continuity.⁵ This feature can imply either that the quantization leads only to the “free” theory, or the quantization leads to the form of a “non-free” theory.

As an example, canonical quantization of $(\varphi^4)_4$ leads only to a “free” theory [7–9], which, incidentally, may lead to unexpected difficulties in the Standard Model (SM). Our quantization of $(\varphi^4)_4$ by affine quantization is a procedure that is just like canonical quantization, after choosing a different pair of classical variables to promote to operators, and can fit well with other quantization procedures, as is implicit in our study.

Affine quantization [13] has offered positive results for several models, one of which includes the nonrenormalizable models $(\varphi^{12})_3$ [14] and $(\varphi^4)_4$ [1].

⁴ The only other similar model is $r = 6$, $n = 3$.

⁵ The paper [12] using ultralocal field models clearly illustrates how the smaller domain wins.

6.2 CQ and AQ of the Covariant Euclidean Field Theory

Canonical quantization has been the go-to method of quantization for many decades. Clearly, the reason for this loyalty is because its use has been so successful. The simple examples from quantum mechanics have led to similar procedures when dealing with field quantization. The formulations of continuous fields can also lead to unwanted divergences. This behavior invites the use of a formal analysis, which addresses selected equations as beacons that regularization of the procedure enables preliminary analysis to occur. This section is devoted to a formal analysis of both canonical and affine quantization of fields initially guided by elementary examples.

For a single classical degree of freedom, the favored variables $-\infty < p, q < \infty$ and a Poisson bracket $\{q, p\} = 1$ lead to the basic quantum operators P, Q , which obey $[Q, P] = i\hbar\mathbb{I}$.

A similar story for classical scalar fields $-\infty < \pi(x), \varphi(x) < \infty$ has a Poisson bracket $\{\varphi(x), \pi(y)\} = \delta^s(x - y)$ which points toward basic quantum operators $\hat{\pi}(x), \hat{\varphi}(x)$, that obeys $[\hat{\varphi}(x), \hat{\pi}(y)] = i\hbar\delta^s(x - y)$. Ideally, the semi-classical action functional for an Euclidean field theory model, $S[\varphi] = \int H[\varphi] dx_0$, is given by

$$S^{(c)}[\varphi] = \int \left\{ \frac{1}{2}[(\nabla\varphi)(x)^2 + m^2\varphi(x)^2] + g\varphi(x)^r \right\} d^n x, \quad (6.6)$$

where the imaginary time x_0 runs from 0 to $\beta = 1/k_B T$ with k_B the Boltzmann constant and T the absolute temperature.

The affine story introduces an important new structure. To see that feature, we return to a single degree of freedom, with p, q . Our analysis instead focuses on the case where $q > 0$. This case implies that the operator $P \neq P^\dagger$. We then seek an operator that can be self adjoint. The new classical variables are $pq, \ln(q)$, which, with $q > 0$, permits each variable to be self adjoint. However, we also need to admit $q < 0$, which can be done when we select unusual classical variables, namely pq, q which permits $-\infty < q \neq 0 < \infty$, and joins together the cases where $q > 0$ and $q < 0$. Affine quantization then involves $pq \rightarrow (P^\dagger Q + QP)/2 \equiv D = D^\dagger$ and $q \rightarrow Q = Q^\dagger$, which obeys $[Q, D] = i\hbar Q$, and already offers a Lie algebra for the “affine group”. Thus, we are led to the *dilation* operator $-\infty < D < \infty$ and the position operator $-\infty < Q \neq 0 < \infty$. This analysis will implicitly be used in discussing the affine quantization of scalar fields.

Consider⁶ $A(x) \times B(x) = C(x)$ as well as $A(x) = C(x)/B(x)$. If $B(x) = C(x) = 0$ what is $A(x)$? If $B(x) = C(x) = \infty$ what is $A(x)$? To ensure getting $A(x)$ one must require $0 < |B(x)| \ \& \ |C(x)| < \infty$. This is good mathematics, but physics has an opinion as well. Consider $\kappa(x) = \pi(x)\varphi(x)$, where $\varphi(x)$ is a chosen physical field, $\pi(x)$ is its momentum field, and their product is $\kappa(x)$, which we will call the dilation field. Since $\pi(x)$ serves as the time derivative of $\varphi(x)$, it can vanish along with $\kappa(x)$. However, requiring that both plus and minus sides of $\varphi(x) \neq 0$

⁶ See Footnote 2.

are acceptable, since the derivative term ensures it will still seem to come from a continuous function. Moreover, if $\varphi(x) = 0$ it could be confused with any other field, e.g., $\alpha(x) = 0$.⁷

It is good math for finite integrations if there are examples where the fields may reach infinity, e.g., $\int_{-1}^1 \varphi^{-2/3} d\varphi < \infty$. However, such cases are very likely to be bad physics because no item of nature reaches infinity. Accepting $\kappa(x) (= \pi(x) \varphi(x))$ and $\varphi(x) \neq 0$, instead of $\pi(x)$ and $\varphi(x)$, as the basic variables, will have profound consequences.

For example, the classical Hamiltonian of Eq. (6.3) in which $0 \leq |\kappa(x)| < \infty$ and $0 < |\varphi(x)| < \infty$, to well represent $\pi(x)$, fulfills the remarkable property that $H(x) < \infty$, where $H[\varphi] = \int H(x) d^s x$, as nature requires! This fact shows that $\kappa(x)$ and $\varphi(x) \neq 0$ should be the new variables!

For an affine field story, we need $\pi(x) \varphi(x) \equiv \kappa(x)$ and $\varphi(x)$, for which $-\infty < \varphi(x) \neq 0 < \infty$, and, as basic operators, $[\hat{\varphi}(x), \hat{\kappa}(y)] = i\hbar \delta^s(x - y) \hat{\varphi}(x)$. Just like the single degree of freedom, we also have the classical relation that $\pi(x)^2 = \kappa(x)^2 / \varphi(x)^2$ as well. However, such a relation does not hold when quantized. In particular, for a single degree of freedom $D Q^{-2} D = P^2 + (3/4)\hbar^2 Q^{-2}$. For the scalar field, the analogous story leads to the relation that $\hat{\kappa}(x) \varphi(x)^{-2} \hat{\kappa}(x) = \hat{\pi}(x)^2 + (3/4)\hbar^2 \delta^{2s}(0) \hat{\varphi}(x)^{-2}$.

In order to explain the extra “3/4” potential term, we use the fact that the operator corresponding to the affine field κ will be the dilation operator $\hat{\kappa} = (\hat{\pi}\hat{\varphi} + \hat{\varphi}\hat{\pi})/2$ where the regularized basic quantum Schrödinger operators are given by $\hat{\varphi}(x) = \varphi(x)$ and $\hat{\pi}(x) = -i\hbar\delta_{\varphi(x)} = -i\hbar\delta/\delta\varphi(x)$ so that the commutator $[\hat{\varphi}(x), \hat{\pi}(y)] = i\hbar\delta^s(x - y)$, where $\delta^s(x)$ is an s -dimensional Dirac delta function since $\delta_{\varphi(x)}\varphi(y) = \delta^s(x - y)$. Multiplying this by $\hat{\varphi}$ we find $[\hat{\varphi}, \hat{\varphi}\hat{\pi}] = [\hat{\varphi}, \hat{\pi}\hat{\varphi}] = [\hat{\varphi}, \hat{\kappa}] = i\hbar\delta^s\hat{\varphi}$ which is only valid for $\varphi \neq 0$. Then $\hat{\kappa} = -i\hbar\{\delta_{\varphi(x)}[\varphi(x)] + \varphi(x)\delta_{\varphi(x)}\}/2 = -i\hbar\{\delta^s(0)/2 + \varphi(x)\delta_{\varphi(x)}\}$. Now, for $\varphi(x) \neq 0$, we will have that affine quantization sends $\hat{\pi}^2(x)$ to

$$\begin{aligned} \hat{\kappa}(x)\varphi^{-2}(x)\hat{\kappa}(x) &= -\hbar^2\{\delta^s(0)/2 + \varphi(x)\delta_{\varphi(x)}\}\varphi^{-2}(x)\{\delta^s(0)/2 + \varphi(x)\delta_{\varphi(x)}\} \\ &= \hbar^2(3/4)\delta^{2s}(0)\varphi^{-2}(x) - \hbar^2\delta_{\varphi(x)}^2 \\ &= \hbar^2(3/4)\delta^{2s}(0)\varphi^{-2}(x) + \hat{\pi}^2(x). \end{aligned} \quad (6.7)$$

The new term involves a Dirac delta function, $\delta(0) = \infty$, raised to the power $2s$. This new formal expression follows the similarly formal expression: $\hat{\pi}(x)^2 = -\hbar^2[\delta^s/\delta\varphi(x)^2]$, wherein such formal terms require regularization, a procedure that we will introduce very soon. The latest relation is featured as an all important semi-classical relation in the following affine action:

⁷ If you think dimensions can distinguish two such fields, we can eliminate dimensional features by first introducing $\varphi(y) \neq 0$ and $\alpha(z) \neq 0$. Now dimensionless factors lead to $\varphi(x)/\varphi(y) = 0 = \alpha(x)/\alpha(z)$. Thus omitting points, or streams of them, where $\varphi(x) = 0$, do not violate any physics.

In fact, it may seem logical to say that $\varphi(x) = 0$ never even belonged in physics. In fact, since numbers were used to count physical things, in very early times, zero = 0, was *banned for 1,500 years*; see [15].

$$S^{(a)}[\varphi] = \int \left\{ \frac{1}{2}[(\nabla\varphi)(x)^2 + m^2 \varphi(x)^2] + g \varphi(x)^r + \frac{3}{8}\hbar^2 \frac{\delta^{2s}(0)}{\varphi(x)^2} \right\} d^n x. \quad (6.8)$$

Once again the origin of $\delta^s(0) = \infty$ is simply the fact that $[\widehat{\varphi}(x), \widehat{\pi}(x)] = i\hbar \delta^s(0) \mathbb{1}$. In a sense, this result is strange. For example, for a single classical variable $(pq)^2 < \infty$ and $|QP - PQ|^2 = \hbar^2 \mathbb{1}$. However, for a classical field $(\pi(x) \varphi(x))^2 < \infty$, while $|\widehat{\varphi}(x) \widehat{\pi}(x) - \widehat{\pi}(x) \widehat{\varphi}(x)|^2 = \infty \hbar^2 \mathbb{1}$. When approximated, as for an integration, then $\widehat{\varphi}(x) \rightarrow \widehat{\varphi}_k$ and $\widehat{\pi}(x) \rightarrow \widehat{\pi}_k$, where instead of the continuum that x represents, k identifies different points on a discrete lattice. This leads to $[\widehat{\varphi}_k, \widehat{\pi}_k] = i\hbar a^{-s} \mathbb{1}$, where a is a tiny spatial distance between neighboring lattice points. In preparation for our integration, just as every integral involves a continuum limit of an appropriate summation, these expressions are used in Monte Carlo (MC) calculations which involve proper sums for their “integrals”. All of this is designed to provide a path integral quantization, and, when necessary, their sums need to be regularized. In our case, the regularized version becomes appropriately “scaled”: specifically $\varphi_k \rightarrow a^{-s/2} \varphi_k$, $\pi_k \rightarrow a^{-s/2} \pi_k$, $\kappa_k \rightarrow a^{-s} \kappa_k$, $g \rightarrow a^{s(r-2)/2} g$, and the regularized $d^s x \rightarrow a^s$ may also be scaled as $a^s \rightarrow a^{2s}$.

6.3 Some Covariant Field Theory Examples

So far, we saw how AQ is able to treat the restricted field space $\varphi > 0$ or $\varphi < 0$.

Here⁸, we review some covariant field theories with an AQ with a restriction of the field space of the kind $\varphi^2 - b^2 > 0$ or $\varphi^2 - b^2 < 0$ with b a real number.

6.3.1 Some Relations Involving the Quantum Operators P , Q , and D

We need $[Q, P] = i\hbar \mathbb{1}$, $F = F(Q) \neq 0$, and we define $D = [PF + FP]/2$, so that $P^\dagger F = PF$.⁹ Then we examine

$$\begin{aligned} 2[F, D] &= F(PF + FP) - (PF + FP)F \\ &= FPF + FFP - PFF - FPF = FFP - PFF = [F^2, P]. \end{aligned} \quad (6.9)$$

This leads to $[F, D] = [F^2, P]/2 = i\hbar(F^2)'/2$, where the prime denotes a derivative with respect to Q . As a familiar example, choose $F(Q) = Q$, then $[Q, D] =$

⁸ Much of the material in this section has been extracted from our Ref. [16].

⁹ As affine quantization permits, the *dilation* operator, D , may take different forms, namely, $D = [PF(Q) + F(Q)P]/2$, for a variety of $F(Q) \neq 0$ functions—chosen such that $P^\dagger F(Q) = PF(Q)$ —and which are of assistance in solving various problems.

$[Q^2, P]/2 = i\hbar(Q^2)'/2 = i\hbar Q$, analogues to the Lie algebra of the affine group, and from which affine quantization got its name.

6.3.2 The Kinetic Factor in Hamiltonians

In simple problems, the most commonly chosen classical kinetic factor is p^2 . In that realm, we can choose $f(q) = 1/g(q) \neq 0$ ($g(q) \neq 0$ is added because $1/f(q)$ is very often used). Now we define $d = pf(q)$ and we then recover p^2 from $d^2 g^2 = d^2/f^2 = p^2$. Admittedly, this is utterly trivial. However, when we quantize these variables to P , $D = (PF + FP)/2$, $F = F(Q) \neq 0$ and $G = G(Q) = 1/F(Q) \neq 0$, difficulties can arise.

The quantum kinetic term (with $\hbar = 1$) in affine variables is DG^2D . This expression, helped by $FP - PF = iF'$ and $GP - PG = iG'$, leads to

$$\begin{aligned} 4DG^2D &= (PF + FP)GG(PF + FP) = PP + FPGGPF + FPGP + PGPF \\ &= PP + (PF + iF')GG(FP - iF') + (PF + iF')GP + PG(FP - iF') \\ &= 4PP + 2i(F'GP - PGF') + F'GGF' = 4PP - 2(F'G)' + (F')^2G^2 \end{aligned} \quad (6.10)$$

Restoring $\hbar$, it follows that

$$DG^2D = P^2 + (1/4)\hbar^2[(F')^2G^2 - 2(F'G)']. \quad (6.11)$$

As a check on this expression, the example in which $F(Q) = Q$ and thus $G(Q) = 1/Q$, leads to $P^2 + (3/4)\hbar^2/Q^2$, which is the result previously found when $F(Q) = Q$. There is every reason to accept this latter equation as the proper kinematical operator for the half-harmonic oscillator [17–19].

6.3.3 Applications

As our first example [16], we choose the classical canonical kinematic field $\pi(x)^2$, for which we choose the *dilation* field $\kappa(x) = \pi(x)\varphi(x)$, with $\varphi(x) \neq 0$. The classical Hamiltonian in affine variables is

$$H_1 = \int \left\{ \frac{1}{2}[\kappa(x)^2/\varphi(x)^2 + (\nabla\varphi)(x)^2 + m^2\varphi(x)^2] + g\varphi(x)^r \right\} d^s x, \quad (6.12)$$

where $r = 4, 6, 8, \dots$ is the interaction power and $n = s + 1$ is the number of space-time dimensions. The advantage of this pair of variables is that $0 < \varphi(x)^{-2} < \infty$

which implies that $0 < \varphi(x)^r < \infty$, for all r , and thus the Hamiltonian does not experience any nonrenormalizability.

Adopting the message from the half-harmonic oscillator, the affine quantum Hamiltonian for this model is

$$\mathcal{H}_1 = \int \left\{ \frac{1}{2} [\widehat{\kappa}(x) \widehat{\varphi}(x)^{-2} \widehat{\kappa}(x) + (\nabla \widehat{\varphi})(x)^2 + m^2 \widehat{\varphi}(x)^2] + g \widehat{\varphi}(x)^r \right\} d^s x, \quad (6.13)$$

in which

$$\widehat{\kappa}(x) \widehat{\varphi}(x)^{-2} \widehat{\kappa}(x) = \widehat{\pi}(x)^2 + (3/4) \hbar^2 \delta(0)^{2s} / \varphi(x)^2. \quad (6.14)$$

With first using CQ for the next example, our next classical Hamiltonian is given by

$$H_2 = \int \left\{ \frac{1}{2} [\pi(x)^2 + (\nabla \varphi)(x)^2 + m^2 \varphi(x)^2] + g (\varphi(x)^2 - \Phi^2)^r \right\} d^s x, \quad (6.15)$$

where the interaction power has been changed to $r = 2, 4, 6, \dots$, and $n = s + 1$ is the same as before. This unusual interaction term deserves a new *dilation* variable,¹⁰ and, in this section, we choose $\kappa(x) = \pi(x) (\varphi(x)^2 - \Phi^2)$, where $(\varphi(x)^2 - \Phi^2) \neq 0$. In this case, the classical Hamiltonian in affine variables becomes

$$H_3 = \int \left\{ \frac{1}{2} [\kappa(x)^2 / (\varphi(x)^2 - \Phi^2)^2 + (\nabla \varphi)(x)^2 + m^2 \varphi(x)^2] + g (\varphi(x)^2 - \Phi^2)^r \right\} d^s x, \quad (6.16)$$

In these variables, $0 < (\varphi(x)^2 - \Phi^2)^{-2} < \infty$, which implies that $0 < (\varphi(x)^2 - \Phi^2)^r < \infty$, for all r , thereby eliminating any nonrenormalizability.

Next we find that the quantum Hamiltonian, using affine variables and Schrödinger's representation, is given by

$$\mathcal{H}_3 = \int \left\{ \frac{1}{2} [\widehat{\kappa}(x) (\varphi(x)^2 - \Phi^2)^{-2} \widehat{\kappa}(x) + (\nabla \varphi)(x)^2 + m^2 \varphi(x)^2] + g (\varphi(x)^2 - \Phi^2)^r \right\} d^s x, \quad (6.17)$$

and this expression will become more useful after the kinetic term is fully analyzed. In order to obtain a valid quantum Hamiltonian for this model, we are first drawn back to Eq. (6.11) in Sect. 6.3.2, which reads $DG^2D = P^2 + (1/4)\hbar^2[(F')^2G^2 - 2(F'G)']$. In the present case, temporally ignoring (x) and still using Schrödinger's representation, $F = (\varphi^2 - \Phi^2)$ and $G = 1/F$. It follows, that $F' = 2\varphi$ and $G' = -2\varphi/(\varphi^2 - \Phi^2)^2$. We also need $(F')^2G^2 = 4\varphi^2/(\varphi^2 - \Phi^2)^2$ and $-2(F'G)' = -4/(\varphi^2 - \Phi^2) + 8\varphi^2/(\varphi^2 - \Phi^2)^2 = 4(\varphi^2 + \Phi^2)/(\varphi^2 - \Phi^2)^2$. Hence, for this model, the kinematic factor is

¹⁰ Being able to change the dilation variable is an important feature of affine quantization.

$$\widehat{\kappa}(x)(\varphi(x)^2 - \Phi^2)^{-2}\widehat{\kappa}(x) = \widehat{\pi}(x)^2 + \hbar^2\delta^{2s}(0)(2\varphi(x)^2 + \Phi^2)/(\varphi(x)^2 - \Phi^2)^2. \quad (6.18)$$

As was the case in Sect. 3.1, scaling can eliminate the $\delta^{2s}(0)$ factor by including the additional scaling factor $\Phi^2 \rightarrow a^{-s}\Phi^2$, and changing the scaling of g to $g \rightarrow a^{s(r-1)}g$.

Using such scaling, in an AQ formulation with MC, has led to a “non-free” result for the scalar field $(\varphi^4)_4$ [20, 21]. However, a CQ formulation with MC, along with analytic studies, has led to a “free” result [1, 7–10, 22].

6.4 Ultralocal Field Theory

We also studied ultralocal field theories¹¹ which differ from the covariant one in that no spatial derivatives in the field are present in the Hamiltonian.

Let us begin with the classical Hamiltonian for a single ultralocal field $\varphi(x)$

$$H(\pi, \varphi) = \int \left\{ \frac{1}{2}[\pi(x)^2 + m^2 \varphi(x)^2] + g |\varphi(x)|^r \right\} d^s x, \quad (6.19)$$

where s is the number of spatial variables and r is any real number. When g is zero, the remaining expression involves a domain in which a full set of variables, i.e., $\pi(x)$ and $\varphi(x)$, lead to a finite Hamiltonian value. If $g = 0 \rightarrow g > 0$, there are two possible results. If $r < 2$, then the domain remains the same. However, if $r > 2$, then there is a new domain that is smaller than the original domain because the interaction term $\int |\varphi(x)|^r d^s x = \infty$ leads to a reduction of certain fields. Since we work in a finite volume region, the fields that cause that divergence are not $\varphi(x) = \infty$, because that would have eliminated the original domain when $g = 0$. The only way for $\int |\varphi(x)|^r d^s x = \infty$ is, for example, given by $\varphi(x) = 1/|x - c|^k$ where k is small enough so that $\int \varphi(x)^2 d^s x < \infty$, while $r > 2$ is big enough so that $\int |\varphi(x)|^r d^s x = \infty$, for example, for $r = 5/2$. Such behavior leads to immediate results in perturbation infinities in a power series of g , leading to a nonrenormalizable process, for which quantum efforts, using canonical quantization, collapse to “free” results, despite that $g > 0$, as all that is continuously connected to the original free theory where $g = 0$. Here we should be more precise since the relevant quantity to look at is the action rather than the Hamiltonian, so we should really compare the interaction term $\int |\varphi(x)|^r d^n x$ and the kinetic term $\int [\partial\varphi(x)/\partial x_0]^2 d^n x$ or the mass term $\int \varphi(x)^2 d^n x$. If we consider stationary fields as particular cases, then the relevant integral is the mass term and we immediately see that we may have triviality for $r > 2$. But the same remains true also for space independent fields.¹²

¹¹ Much of the material in this section is extracted from our Ref. [3].

¹² If we consider $\varphi(x) = 1/|x_0 - c|^k$ then in order to have $\mathcal{D}_{g>0} \subset \mathcal{D}_{g=0}$, where $\mathcal{D}_g$ is the domain of those $\varphi(x)$, in the ultralocal theory, where the action is not divergent, we require a divergent

The classical affine variables are the *dilation* $\kappa(x) \equiv \pi(x) \varphi(x)$ and the field $\varphi(x) \neq 0$. The reason we insist that $\varphi(x) \neq 0$ is because if $\varphi(x) = 0$ and $\kappa(x) = 0$ then $\pi(x)$ is not well defined.

We next introduce the same classical Hamiltonian we chose before now expressed in affine variables. This leads us to

$$H'(\kappa, \varphi) = \int \left\{ \frac{1}{2} [\kappa(x)^2 \varphi(x)^{-2} + m^2 \varphi(x)^2] + g |\varphi(x)|^r \right\} d^s x, \quad (6.20)$$

in which $\varphi(x) \neq 0$ is an important fact. With these variables, we see that $\pi = \kappa/\varphi$ so we should not let neither $\varphi = 0$ nor $\varphi = \pm\infty$; otherwise in either cases, we could find a form of indecision ($0/0$ or ∞/∞) for the *dilation* κ which would then be not well defined.¹³ The essential result $0 < |\varphi(x)| < \infty$, leads to the fact that these AQ bounds on $\varphi(x)$ *forbid any nonrenormalizability*, a “disease” which plagues the CQ analysis. With AQ, this new insight implies that any model $(\varphi^r)_n$ does not become a “free” result, but leads to an appropriate “non-free” result.

The quantum affine operators are the scalar field $\hat{\varphi}(x) = \varphi(x)$ and the *dilation* operator¹⁴ $\hat{\kappa}(x) = [\hat{\varphi}(x)\hat{\pi}(x) + \hat{\pi}(x)\hat{\varphi}(x)]/2$ where the momentum operator is $\hat{\pi}(x) = -i\hbar\delta/\delta\varphi(x)$. Accordingly for the self-adjoint kinetic term, $\hat{\kappa}(x)\hat{\varphi}(x)^{-2}\hat{\kappa}(x) = \hat{\pi}(x)^2 + (3/4)\hbar\delta(0)^{2s}\varphi(x)^{-2}$ and one finds for the quantum Hamiltonian operator

$$\hat{H}'(\hat{\kappa}, \hat{\varphi}) = \int \left\{ \frac{1}{2} [\hat{\pi}(x)^2 + m^2 \varphi(x)^2] + g |\varphi(x)|^r + \frac{3}{8}\hbar^2 \frac{\delta(0)^{2s}}{\varphi(x)^2} \right\} d^s x. \quad (6.21)$$

As in previous works [20, 21, 23], we use the scaling $\pi \rightarrow a^{-s/2}\pi$, $\varphi \rightarrow a^{-s/2}\varphi$, $g \rightarrow a^{s(r-2)/2}g$, which is necessary¹⁵ to eliminate the Dirac delta factor $\delta(0) = a^{-1}$ divergent in the continuum limit $a \rightarrow 0$.

In Ref. [3], we studied with path integral Monte Carlo the ultralocal Euclidean scalar field theory $(\varphi^4)_2$ quantized through scaled affine and canonical quantization. Note that in this case the requirement $r > 2$ implies that the scaling factor for the bare

interaction term but a convergent kinetic term or $rk > 1 > 2(k+1)$ that is possible if $r > -2$. Additionally, since we always want a convergent mass term we must also have $0 < k < 1/2$ which again requires $r > 2$ for triiviality. This means that for $r > 2$ the domains change because of reducing g back to zero will only retain the smallest version of the domain by continuity, and that will not be the theory you started out with. For space independent fields, the ultralocal theory is the same as the covariant theory which is trivial for $r > 2n/(n-2) > 2$. This is due to the fact that $\mathcal{D}_g^{\text{covariant}} \neq \mathcal{D}_g^{\text{ultralocal}}$.

¹³ See Footnote 2.

¹⁴ Since $\varphi(x) \neq 0$, that means $\pi^\dagger \neq \pi$ so, to make that clear we should say that $\hat{\kappa}(x) \equiv [\hat{\varphi}(x)\hat{\pi}(x) + \hat{\pi}^\dagger(x)\hat{\varphi}(x)]/2$ to make sure that $\hat{\kappa}^\dagger = \hat{\kappa}$. But $\hat{\pi}^\dagger\hat{\varphi} = \hat{\pi}\hat{\varphi}$ because in that case $\hat{\pi}^\dagger$ acts like $\hat{\pi}$ thanks to having $\hat{\pi}$ acting on $\hat{\varphi}$.

¹⁵ Note that from a physical point of view one never has to worry about the mathematical divergence since the lattice spacing will necessarily have a lower bound. For example at an atomic level, one will have $a \gtrsim 1\text{\AA}$. In other words, the continuum limit will never be a mathematical one.

coupling constant, $a^{s(r-2)/2}$, tends to zero in the continuum limit $a \rightarrow 0$. Therefore the requirement that the scaled coupling remains finite implies a “free” unscaled theory.

Our numerical results show clearly how in the AQ case at least in a neighborhood of a small bare coupling constant the renormalized coupling constant does not tend to zero in the continuum limit. This is sufficient to conclude that the $(\varphi^4)_2$ theory treated with AQ is nontrivial.

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Chapter 7

Path Integral Monte Carlo



*e poscia per lo ciel, di lume in lume,
ho io appreso quel che s'io ridico,
a molti fia sapor di forte agrume;*

*Dante Alighieri
La Divina Commedia (canto XVII paradiso)*

Abstract In this chapter, we describe the Path Integral Monte Carlo method used to study the various Canonical and Affine Quantized field theories previously introduced and present some of the numerical results obtained in our Numerical Experiments.

In this chapter, we present in a unified way the Path Integral Monte Carlo (PIMC) method used to study the *real* scalar field theories φ_n^r presented in the previous Chap. 6. In the last section, we present our numerical results from the various computer experiments for the covariant $r = 12, n = 3$ and $r = 4, n = 4$. For the ultralocal $r = 4, n = 2$, we refer the reader to Sect. 6.4 and our Ref. [1].

In the next Chap. 8, we applied PIMC to a particular *complex* scalar field in order to study the Higgs Mexican hat case (see Chap. 3 and Fig. 3.2) as a standalone presentation.

7.1 Lattice Field Theory

The theory considers a real scalar field φ taking the value $\varphi(x)$ on each site of a periodic n -dimensional lattice, with $n = s + 1$ spacetime dimensions, of lattice spacing a , the ultraviolet cutoff, and spatial periodicity $L = Na$ and temporal periodicity $\beta = N_0 a$. The field path is a closed loop on an n -dimensional surface of an $(n + 1)$ -dimensional β -cylinder. We introduce a lattice formulation of the AQ covariant field theory of Eq. (6.8) (also studied in Eq. (8) of [2] and Eq. (5) of [3]) using the scaling $\varphi \rightarrow a^{-s/2} \varphi$ and $g \rightarrow a^{s(r-2)/2} g$ which is necessary to eliminate the Dirac delta

factor $\delta(0) = a^{-1}$ divergent in the continuum limit $a \rightarrow 0$. The affine action for the field, in the *primitive approximation* [4], is then approximated by

$$\mathcal{S}^a[\varphi]/a = \frac{1}{2} \left\{ \sum_{x,\mu} a^{-2} [\varphi(x) - \varphi(x + e_\mu)]^2 + m^2 \sum_x \varphi(x)^2 \right\} + \sum_x g \varphi(x)^r + \frac{3}{8} \sum_x \frac{\hbar^2}{\varphi(x)^2}, \quad (7.1)$$

where e_μ is a vector of length a in the $+\mu$ direction with $\mu = 0, 1, 2, \dots, s$. In this expression for $\mathcal{S} = \mathcal{K} + \mathcal{V}$, the first sum is the kinetic energy part $\mathcal{K}$, which contributes to a continuous path, and all the rest (the next three sums) are the potential energy part $\mathcal{V}$ or the self-interaction terms. We will have $S^a \approx \mathcal{S}^a$. The primitive approximation for the unscaled CQ action, $\mathcal{S}^c$ will be obtained removing from Eq. (7.1) the last term (the one with the $\frac{3}{8}$ factor), up to a factor a^s .

We will use this “primitive approximation” for the action even if it can be improved in several ways [4] in order to reduce the error due to the spacetime discretization. In reaching to the expression (7.1), we neglected the term $\propto a^{2n}$ due to the commutator of the kinetic and potential parts of the Hamiltonian, in the Baker-Campbell-Hausdorff formula. In reaching to the path integral expression, this is justified by the Trotter formula.

We are interested in reaching the *continuum limit* by taking $L = Na$ fixed and letting $N \rightarrow \infty$ at fixed volume L^s . As for the temporal periodicity, we can initially treat it on the same footing of the spatial periodicity taking $\beta = L$ and $N_0 = N$ as was done in the following Refs. [1, 2, 5–10]. On the other hand, we can distinguish the two periodicities allowing the absolute temperature $T = 1/k_B\beta$ to vary so that the number of discretization points for the imaginary time interval $[0, \beta]$ will be $N_0 = \beta/a$. In Ref. [3], we were, for example, interested in the $N_0 \gg N$ (or $\beta \gg L$) regime.

The vacuum expectation value of an observable $\mathcal{O}[\varphi]$ will then be given by the following expression:

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{O}[\varphi] \exp(-\mathcal{S}[\varphi]) \mathcal{D}\varphi(x)}{\int \exp(-\mathcal{S}[\varphi]) \mathcal{D}\varphi(x)}, \quad (7.2)$$

where $\mathcal{D}\varphi(x) \equiv \prod_x d\varphi(x)$ and the functional integrals will be calculated on a lattice using the path integral Monte Carlo method as explained further on.

7.2 The Monte Carlo Method

The *Monte Carlo method* [11] is a way to estimate numerically a highly multidimensional integral¹ and it is therefore ideally suited to evaluate a path integral. Since field

¹ Which becomes more and more efficient than the usual quadrature methods as the number of dimensions increases. In general, the MC integration becomes more efficient than a grid-based integration as soon as the number of dimensions of the integral is bigger than twice the order of the quadrature integration scheme.

theory reduces to a one-body problem our task has been much simpler than what is usually done in quantum many-body liquids [4]. The material in Sects. 7.2.1, 7.2.2 and 7.2.4 is extracted verbatim from pages 3–8 of the article [12]² and on unpublished lecture notes of a graduate course, given by D. Ceperley, that I attended at the University of Illinois Urbana/Champaign in 1996.

7.2.1 Random Walks

Let us start by reviewing the random walk or equivalently Markov chains. The application of these ideas have led to one of the most important and pervasive numerical algorithm to be used on computers: the *Metropolis* algorithm first used by Metropolis, Rosenbluth, and Teller in 1953 [13], M(RT)². It is a general method of sampling arbitrary highly dimensional probability distributions by taking a random walk through configuration space. Virtually, all Quantum Monte Carlo simulations are done using a generalization of the Metropolis rejection algorithm. The problem is that we want to sample the probability distribution:

$$\pi(s) = \frac{\exp[-S(s)]}{Z}, \quad (7.3)$$

where $S(s)$ is the action. The partition function Z normalizes the function π in this space and is usually not known.

Let us briefly review the properties of Markov chains. In a Markov chain, one changes the state of the system randomly according to a fixed *transition rule*, $\mathcal{P}(s \rightarrow s')$, thus generating a random walk through state space, $\{s_0, s_1, s_2 \dots\}$. The definition of a Markov process is that the next step is chosen for a probability distribution fixed in “time” and depending only on the “present”. This makes it very easy to describe mathematically. The process is often called the drunkard’s walk. $\mathcal{P}(s \rightarrow s')$ is a probability distribution so that it satisfies

$$\sum_{s'} \mathcal{P}(s \rightarrow s') = 1, \quad (7.4)$$

and

$$\mathcal{P}(s \rightarrow s') \geq 0. \quad (7.5)$$

Given a probability distribution function $\pi(s)$, the random walk steps are designed so that when repeated again and again, the asymptotic distribution of s ’s is $\pi(s)$. Each of the s_n is a random variable and has an associated probability $\pi_n(s)$, where $\pi_0(s)$ can be any distribution for s . The $\pi_n(s)$ has the property that asymptotically

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$$\lim_{n \rightarrow \infty} \pi_n(s) = \pi(s). \quad (7.6)$$

According to a theorem in Feller [14], if the transition probability $\mathcal{P}$ is *ergodic*, then an asymptotic probability distribution function $\pi(s)$ exists and is *unique* if $\pi(s)$ is a stationary point of the recursion. That means there is a unique solution to:

$$\sum_s \pi(s) \mathcal{P}(s \rightarrow s') = \pi(s'). \quad (7.7)$$

Then the distribution of s_n converges to a *unique equilibrium state*. Systems defined by random walks can be partitioned into several categories. If, in a random walk, the probability of returning to a neighborhood about s is 0, then the system is called a *null* system and the expected recurrence time is infinite. A system where the random walk will return to the neighborhood of s every T steps is called *periodic*. An ergodic system is one in which the random walk may return to the neighborhood of s but does not do so periodically; it is neither null nor periodic. The transition is ergodic if:

1. One can move from any state to any other state in a finite number of steps with a non-zero probability, i.e., there are no barriers that restrict any walk to a subset of the full configuration space.
2. It is not periodic. Non-periodic rule holds if $\mathcal{P}(s \rightarrow s) > 0$; if there is always some chance of staying put.
3. The average return time to any state is finite. This is always true in a finite system (e.g., periodic boundary conditions). It would be violated in a model of the expanding universe where the system gets further and further from equilibrium because there is no possibility of energy flowing between separated regions after the “big bang”.

Under these conditions, we can show that if $\pi_n(s)$ is the probability distribution of random walks after n steps, with $\pi_0(s)$ the initial condition, then:

$$\pi_n(s) = \pi(s) + \sum_{\lambda} \epsilon_{\lambda}^n \phi_{\lambda}(s), \quad (7.8)$$

where the $0 < \epsilon_{\lambda} < 1$ with ϕ_{λ} some functions. So the probability distribution converges exponentially fast to the stationary distribution π . The convergence is monotonic and the distance between π_n and π is strictly decreasing with $|\pi_n - \pi| > |\pi_{n+1} - \pi|$.

The asymptotic transition probabilities often satisfy the *detailed balance* property: the transition rate from s to s' equals the reverse rate,

$$\pi(s) \mathcal{P}(s \rightarrow s') = \pi(s') \mathcal{P}(s' \rightarrow s), \quad (7.9)$$

If the pair $\{\pi(s), \mathcal{P}(s \rightarrow s')\}$ satisfy detailed balance and if $\mathcal{P}(s \rightarrow s')$ is ergodic, then the random walk must eventually have π as its equilibrium distribution. To

prove this fact, sum the previous equation over s and use Eq. (7.4) to simplify the right-hand side. Detailed balance is one way of making sure that we sample π . It is a sufficient condition. Some methods work directly with the equilibrium Eq. (7.7).

7.2.2 $M(RT)^2$ Algorithm

The Metropolis $M(RT)^2$ (rejection) method is a particular way of ensuring that the transition rule satisfy detailed balance.³ It does this by splitting the transition probability into an “a priori” *sampling probability distribution* $T(s \rightarrow s')$, which we can sample, and an *acceptance probability distribution* $A(s \rightarrow s')$.

$$\mathcal{P}(s \rightarrow s') = T(s \rightarrow s')A(s \rightarrow s'), \quad (7.10)$$

In the Metropolis procedure [11], trial moves are accepted according to⁴:

$$A(s \rightarrow s') = \min[1, q(s' \rightarrow s)], \quad (7.12)$$

where

$$q(s \rightarrow s') = \frac{\pi(s')T(s' \rightarrow s)}{\pi(s)T(s \rightarrow s')} \geq 0. \quad (7.13)$$

It is easy to verify detailed balance and hence asymptotic convergence with this procedure by looking at the three cases: $s = s'$ (trivial), $q(s \rightarrow s') \leq 1$, and $q(s \rightarrow s') \geq 1$. Two common errors are: first, if you can move from state s to s' , then the reverse move must also be possible (both $T(s \rightarrow s')$ and $T(s' \rightarrow s)$ should be zero or non-zero together) and secondly moves that are not accepted are rejected and remain at the same location for at least one more step. Accepted or rejected steps contribute to averages in the same way.

Here is the Metropolis algorithm:

1. Decide what distribution to sample, $\pi(s)$, and how to move from one state to another with the sampling distribution $T(s \rightarrow s')$;
2. Initialize the state: pick s_0 ;
3. To advance the state from s_n to s_{n+1} :
 - i. Sample s' from the sampling distribution $T(s_n \rightarrow s')$

³ $M(RT)^2$ is ergodic [15].

⁴ Other forms are possible, even if not optimal. For example, also

$$A'(s \rightarrow s') = \frac{q(s' \rightarrow s)}{1 + q(s' \rightarrow s)}, \quad (7.11)$$

satisfies detailed balance, since $q(s \rightarrow s')q(s' \rightarrow s) = 1$.

ii. Calculate the ratio:

$$q = \frac{\pi(s')T(s' \rightarrow s_n)}{\pi(s_n)T(s_n \rightarrow s')} \quad (7.14)$$

iii. Accept or reject:

If $q > 1$ or if $q > u_n$ where u_n is a uniformly distributed Random Number (RN) in $(0,1)$ set $s_{n+1} = s'$. Otherwise set $s_{n+1} = s_n$;

4. Throw away the first κ states as being out of equilibrium;

5. Collect averages every so often, and block them [16] to get error bars;

Consider the sampling of a probability distribution, $\exp[-S(s)]$. In the original Metropolis procedure, $T(s \rightarrow s')$ was chosen to be a constant distribution inside a segment (for a scalar field) and zero outside. This is the *classic* rule: a single field at a single lattice point is displaced uniformly, the segment length δ is adjusted to achieve 50% acceptance. Since T is a constant, it drops out of the acceptance formula. So the update rule is $s \rightarrow s'$ and accept or reject based on $\exp[-S(s') + S(s)]$. Moves that lower the action are always accepted. Moves that raise the action are often accepted if the action cost is small. Hence, the random walk does not simply roll downhill. Fluctuations can drive it uphill.

Some things to note about Metropolis:

- One nice feature is that fields can be moved one at a time. And moves involving many fields at different lattice points may become inefficient.
- One needs both the forward probability and the reverse probability if one has a nonuniform transition probability. Also one cannot calculate the normalization of π . It is never needed. Only ratios enter in.
- The acceptance ratio (number of successful moves/total number of trials) is a key quantity to keep track of and to quote. Clearly if the acceptance ratio is very small, one is doing a lot of work without moving through phase space. On the other hand, if the acceptance ratio is close to 1, you could probably try larger steps and get faster convergence. There is a rule-of-thumb that it should be 1/2, but in reality we have to look at the overall efficiency.
- One can show that the Metropolis acceptance formula is optimal among formulas of this kind which satisfy detailed balance.

Since asymptotic convergence is easy to guarantee, the main issue is whether configuration space is explored thoroughly in a reasonable amount of computer time. Let us define a measure of the convergence rate and of the efficiency of a given Markov process. This is needed to compare the efficiency of different transition rules, to estimate how long the runs should be, and to calculate statistical errors. The rate of convergence is a function of the property being calculated. Generally, one expects that there are local properties which converge quickly and other properties (such as order parameters near a phase boundary) which converge very slowly.

Let $\mathcal{O}(s)$ be a given property and let its value at step k of the random walk be $\mathcal{O}_k$. Let the mean and intrinsic variance of $\mathcal{O}$ be denoted by

$$\bar{\mathcal{O}} = \langle \mathcal{O} \rangle \quad (7.15)$$

and

$$\sigma_{\mathcal{O}}^2 = \langle (\mathcal{O}_k - \bar{\mathcal{O}})^2 \rangle \quad (7.16)$$

where the averages $\langle . . . \rangle$ are over π . These quantities depend only on the distribution π , not on the Monte Carlo procedure. In the next Sect. 7.2.4, we show that the standard error of the estimate of the average, $\bar{\mathcal{O}}$, over a Markov chain with P steps, is

$$\text{error}[\bar{\mathcal{O}}] = \sqrt{\frac{\sigma_{\mathcal{O}}^2 \tau_{\mathcal{O}}}{P}}, \quad (7.17)$$

where $\tau_{\mathcal{O}}$ is the *correlation time* defined in Eq. (7.23) where there we called $\mathcal{O} \equiv F$. It gives the average number of steps to decorrelate the property $\mathcal{O}$. The correlation time will depend crucially on the transition rule and has a minimum value of 1 if one can move so far in configuration space that successive values are uncorrelated. In general, the number of independent steps which contribute to reducing the error bar from Eq. (7.17) is not P but P/τ .

Hence to determine the true statistical error in a random walk, one needs to estimate the correlation time. To do this, it is very important that the total length of the random walk be much greater than $\tau_{\mathcal{O}}$. Otherwise, the result and the error will be unreliable. Runs in which the number of steps is $P \gg \tau_{\mathcal{O}}$ are called *well converged*. In general, there is no mathematically rigorous procedure to determine τ . Usually, one must determine it from the random walk. It is a good practice occasionally to run very long runs to test that the results are well converged.

The correlation time defined in Eq. (7.23) is an equilibrium average. There is another correlation time relevant to Markov chains, namely, how many steps it takes to reach equilibrium from some starting state. Normally, this will be at least as long as the equilibrium correlation time, but in some cases, it can be much longer. The simplest way of testing convergence is to start the random walk from several, radically different, starting places and see if a variety of well-chosen properties converge to the same values. Metastability and hysteresis are characteristic near a (first-order) phase boundary. A random starting place is with placing each variable randomly in the total space. It may be very difficult for the system to go to the equilibrium distribution from this starting place.

The *efficiency* of a random walk procedure, for the property $\mathcal{O}$, is defined as how quickly the errors bars decrease as a function of computer time,

$$\xi_{\mathcal{O}} = \frac{1}{\sigma_{\mathcal{O}}^2 \tau_{\mathcal{O}} T}, \quad (7.18)$$

where T is the computer time per step. Hence, the efficiency is independent of the length of the calculation and is the figure-of-merit for a given algorithm. The

efficiency depends not only on the algorithm but also on the computer and the implementation. Methods that generate more steps per hour are, other things being equal, more efficient. We are fortunate to live in a time when the efficiency is increasing because of rapid advances in computers. Improvements in algorithms can also give rise to dramatic increases in efficiency. If we ignore how much computer time a move takes, an optimal transition rule is one which minimizes $\tau_{\mathcal{O}}$, since $\sigma_{\mathcal{O}}^2$ is independent of the sampling algorithm.

Usually, transition rules are local. At a given step, only a few fields are moved. If we try to move too many variables simultaneously, the move will almost certainly be rejected, leading to long correlation times.

7.2.3 Application to Our Lattice Field Theory Problem

The MC simulation (or computer experiment) use the Metropolis algorithm [11, 13] to calculate the discretized version of Eq. (7.2) which is an N^n multidimensional integral. So clearly, the computational resources needed to perform a given simulation depends critically on n . At high n , it will cost more to approach the continuum limit $N \rightarrow \infty$. We always use natural Planck units $c = \hbar = k_B = 1$. The simulation is started from any initial condition. One MC step consisted in a random displacement of each one of the N^n components of φ as follows

$$\varphi \rightarrow \varphi + (2\eta - 1)\delta, \quad (7.19)$$

where η is a uniform pseudo-random number in $[0, 1]$ and δ is the amplitude of the displacement. Each one of these N^n moves is accepted if $\exp(-\Delta\mathcal{S}) > \eta$ where $\Delta\mathcal{S}$ is the change in the action due to the move (it can be efficiently calculated considering how the kinetic part and the potential part change by the displacement of a single component of φ) and rejected otherwise. The amplitude δ is chosen in such a way to have acceptance ratios as close as possible to $1/2$ and is kept constant during the evolution of the simulation. One simulation consisted of a large number of p steps. The statistical error on the average $\langle F \rangle$ will then depend on the correlation time, τ_F , necessary to decorrelate the property F and will be determined as $\sqrt{\sigma_F^2 \tau_F / (pN^n)}$, where σ_F^2 is the intrinsic variance for F , as shown in Sect. 7.2.4.

Our estimate of the path integrals will be generally subject to three sources of numerical uncertainties: The one due to the statistical error, the one due to the space-time discretization, and the one due to the finite-size effects. Of these, the statistical error scales like $P^{-1/2}$ where $P = pN^n$ is the computer time, the discretization of spacetime is responsible for the distance from the continuum limit (which corresponds to a lattice spacing $a \rightarrow 0$), and the finite-size effects stems from the necessity to approximate the infinite spacetime system with one in a periodic box of volume L^n with $L = Na$ being the box side made of N discretization points.

7.2.4 Estimating the Statistical Error

Let F be a given property and let its value at step k of the random walk be F_k . Let the mean and intrinsic variance of F be denoted by

$$\bar{F} = \langle F_k \rangle = \frac{1}{P} \sum_{k=1}^P F_k \quad (7.20)$$

and

$$\sigma_F^2 = \langle (F_k - \bar{F})^2 \rangle \quad (7.21)$$

These quantities depend only on the distribution $e^{-S} / \int e^{-S}$, not on the Monte Carlo procedure. We can show that the standard error of the estimate of the average, $\bar{F}$, over a Markov chain with P steps, is

$$\text{error}[\bar{F}] = \sqrt{\left\langle \left(\frac{1}{P} \sum_{k=1}^P F_k - \frac{1}{P} \sum_{k=1}^P \bar{F} \right)^2 \right\rangle} = \sqrt{\frac{\sigma_F^2 \tau_F}{P}}. \quad (7.22)$$

where τ_F is the *correlation time* that can be estimated as follows

$$\tau_F \approx 1 + 2 \sum_{k=1}^P \frac{\langle (F_0 - \bar{F})(F_k - \bar{F}) \rangle}{\sigma_F^2}, \quad (7.23)$$

and it gives the average number of steps to decorrelate the property F which has a minimum value of 1 if one can move so far in configuration space that successive values are uncorrelated. In general, the number of independent steps which contribute to reducing the error bar from Eq. (7.22) is not P but P/τ . An alternative way to estimate the correlation time is through data blocking as shown in Ref. [16].

7.3 Renormalized Quantities and Relevant Observables

On the lattice⁵

$$\int \dots d^n x \rightarrow a^n \sum_n \dots \quad \text{and} \quad \delta(x) \rightarrow a^{-n} \delta_x, \quad (7.24)$$

where $\delta(x)$ is a Dirac delta and δ_x is a Kronecker delta. The coefficients of the Fourier series of the field on the periodic lattice are

⁵ Much of this section has been extracted from our Ref. [6].

$$\tilde{\varphi}(p) = \int_{L^n} \varphi(x) e^{ip \cdot x} d^n x \rightarrow \sum_n \varphi(x) e^{ip \cdot x} a^n, \quad (7.25)$$

with $p = (2\pi/L)k$ with $k_\mu \in \mathbb{Z}$ and $\mu = 0, 1, \dots, s$. And the Fourier series

$$\varphi(x) = L^{-n} \sum_k \tilde{\varphi}(p) e^{-ip \cdot x}. \quad (7.26)$$

Note that

$$\int_{L^n} e^{ip \cdot x} d^n x = L^n \delta_k. \quad (7.27)$$

For $L \rightarrow \infty$, one finds the Fourier transform

$$\varphi(x) \rightarrow \int \tilde{\varphi}(p) e^{-ip \cdot x} \frac{d^n p}{(2\pi)^n} \quad \text{and} \quad L^{-n} \sum_k e^{-ip \cdot x} \rightarrow \delta(x). \quad (7.28)$$

Now, choosing e_μ with all its components equal to zero except one, we find

$$\begin{aligned} (\nabla \varphi)(x)^2 &\rightarrow \left(\sum_\mu \frac{\varphi(x) - \varphi(x + e_\mu)}{a} \right)^2 \\ &= \int \frac{d^n p}{(2\pi)^n} \int \frac{d^n q}{(2\pi)^n} e^{-i(p+q) \cdot x} \left(\frac{1 - e^{-ipa}}{a} \right) \left(\frac{1 - e^{-iq a}}{a} \right) \tilde{\varphi}(p) \tilde{\varphi}(q) \\ &= -4a^{-2} \int \frac{d^n p}{(2\pi)^n} \int \frac{d^n q}{(2\pi)^n} e^{-i(p+q) \cdot (x-a/2)} \sin(pa/2) \sin(qa/2) \tilde{\varphi}(p) \tilde{\varphi}(q). \end{aligned} \quad (7.29)$$

Using $\int e^{ip \cdot x} d^n x = (2\pi)^n \delta(p)$ for $L \rightarrow \infty$ and $\tilde{\varphi}(-p) = \tilde{\varphi}(p)^*$ for a real scalar field $\varphi(x)$, we also have

$$\int (\nabla \varphi)(x)^2 d^n x = 4a^{-2} \int \frac{d^n p}{(2\pi)^n} \sin^2(pa/2) |\tilde{\varphi}(p)|^2, \quad (7.30)$$

$$\int \varphi(x)^2 d^n x = \int \frac{d^n p}{(2\pi)^n} |\tilde{\varphi}(p)|^2. \quad (7.31)$$

7.3.1 Renormalized Mass

We define a renormalized mass

$$m_R^2 = \frac{p^2 \langle |\tilde{\varphi}(p)|^2 \rangle}{\langle \tilde{\varphi}(0)^2 \rangle - \langle |\tilde{\varphi}(p)|^2 \rangle}, \quad (7.32)$$

where the momentum p has all components equal to zero except one. Then

$$\langle |\tilde{\varphi}(p)|^2 \rangle = \frac{\int \mathcal{D}\tilde{\varphi} |\tilde{\varphi}(p)|^2 e^{-S[\tilde{\varphi}]}}{\int \mathcal{D}\tilde{\varphi} e^{-S[\tilde{\varphi}]}}, \quad (7.33)$$

Now, using Eq. (7.30), we find for a “free” ($g \rightarrow 0$) CQ field theory

$$S[\tilde{\varphi}] = \int \frac{d^n p}{(2\pi)^2} \frac{1}{2} \left[\frac{4}{a^2} \sin^2(pa/2) + m^2 \right] |\tilde{\varphi}(p)|^2, \quad (7.34)$$

so that

$$\langle |\tilde{\varphi}(p)|^2 \rangle = \frac{1}{\frac{4}{a^2} \sin^2(pa/2) + m^2}, \quad (7.35)$$

where we used the following Gaussian integration:

$$I(\alpha) = \int e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}, \quad (7.36)$$

$$-I'(\alpha) = \int x^2 e^{-\alpha x^2} dx = (1/2\alpha) \sqrt{\pi/\alpha}. \quad (7.37)$$

So we find

$$\begin{aligned} m_R^2 &= \frac{p^2}{\frac{1/m^2}{1/\left[\frac{4}{a^2} \sin^2(pa/2) + m^2\right]} - 1} \\ &= m^2 \frac{(pa/2)^2}{\sin^2(pa/2)} \xrightarrow{a \rightarrow 0} m^2, \end{aligned} \quad (7.38)$$

where m is the bare mass. Of course $\lim_{g \rightarrow 0, a \rightarrow 0} m_R^2 \neq m^2$ in AQ.

7.3.2 Renormalized Coupling

We define a renormalized coupling constant

$$g_R = 3 - \frac{\langle \tilde{\varphi}(0)^4 \rangle}{\langle \tilde{\varphi}(0)^2 \rangle^2}. \quad (7.39)$$

Note that $\lim_{g \rightarrow 0} g_R = 0$, where g is the bare coupling constant. In fact for a “free” ($g \rightarrow 0$) CQ field theory, we immediately find (see previous subsection)

$$\frac{\langle \tilde{\varphi}(0)^4 \rangle}{\langle \tilde{\varphi}(0)^2 \rangle^2} = 3, \quad (7.40)$$

using the additional Gaussian integration (see Eq. (7.36))

$$I''(\alpha) = \int x^4 e^{-\alpha x^2} dx = (3/4\alpha^2) \sqrt{\pi/\alpha}. \quad (7.41)$$

Of course $\lim_{g \rightarrow 0} g_R \neq 0$ in AQ.

7.3.3 The n -Points Functions

Let's start with the two-point connected function (the Green function)

$$K(x, y) = [\langle \varphi(x) \rangle - \langle \varphi(x) \rangle][\langle \varphi(y) \rangle - \langle \varphi(y) \rangle] = \langle \varphi(x) \varphi(y) \rangle - \langle \varphi(x) \rangle^2. \quad (7.42)$$

Using translational invariance of the theory and assuming a vanishing vacuum expectation value of the field $\langle \varphi(x) \rangle = 0$, we can also define (remember that $L = Na$)

$$\begin{aligned} \bar{D}(z) &= \frac{1}{N^n} \sum_x K(x, x+z) \\ &= \frac{1}{N^n L^{2n}} \sum_x \sum_k \sum_{k'} \langle \tilde{\varphi}(p) \tilde{\varphi}(p') \rangle e^{ip \cdot x} e^{ip' \cdot (x+z)} \\ &= \frac{1}{L^n} \sum_k \sum_{k'} \delta_{k+k'} \langle \tilde{\varphi}(p) \tilde{\varphi}(p') \rangle e^{ip' \cdot z} \\ &= \frac{1}{L^n} \sum_k \langle |\tilde{\varphi}(p)|^2 \rangle e^{-ip \cdot z}. \end{aligned} \quad (7.43)$$

For a “free” ($g \rightarrow 0$) CQ field theory of mass m in the $L \rightarrow \infty$ limit and in the continuum limit $a \rightarrow 0$, we then find

$$\bar{D}(z) = \int \frac{d^n p}{(2\pi)^n} \frac{e^{-ip \cdot z}}{p^2 + m^2} = m K_1(m|z|)/|z|4\pi^2, \quad (7.44)$$

where K_1 is a modified Bessel function. For the massless $m = 0$ case

$$\bar{D}(z) = \int \frac{e^{-ip \cdot z}}{p^2} \frac{d^n p}{(2\pi)^n} = \begin{cases} -|z|/2 & n = 1 \\ -(\ln |z|/l)/2\pi & n = 2 \\ 1/|z|4\pi & n = 3 \\ 1/|z|^2 4\pi^2 & n = 4 \end{cases}, \quad (7.45)$$

where $|z| = \sqrt{z_0^2 + z_1^2 + \dots + z_s^2}$ and l is a length. This shows how the massless field generates long-range interactions.

In periodic spacetime (at a temperature $T = 1/Na$)

$$D(z) = \sum_{w_n} \bar{D}(z + Lw_n), \quad (7.46)$$

with $w_n = (n_0, n_1, \dots, n_s)$ and $n_\mu \in \mathbb{Z}$. The sum can be restricted by an infrared cutoff irc such that $-irc \leq n_\mu \leq irc$ (without any physical significance) in order to reach a given numerical accuracy. If we remove the cutoff, the function diverges for the massless case.

One usually defines all the other n -points functions introducing the generating functional $J[t] = \exp[\int t(x)\varphi(x) dx]$ so that

$$J[t] = 1 + \sum_{n=1}^{\infty} \int \dots \int \frac{t(x_1) \dots t(x_n)}{n!} \varphi(x_1) \dots \varphi(x_n) dx_1 \dots dx_n, \quad (7.47)$$

to find

$$\langle J[t] \rangle = 1 + \sum_{n=1}^{\infty} \int \dots \int \frac{t(x_1) \dots t(x_n)}{n!} \mu_n(x_1, \dots, x_n) dx_1 \dots dx_n,$$

where $\mu_n(x_1, \dots, x_n) = \langle \varphi(x_1) \dots \varphi(x_n) \rangle$ is the n -points function or n -moment. It is interesting to remember here that another set of useful functions are the n -cumulants $k_n(x_1, \dots, x_n)$ defined through the other generating functional

$$C[t] = \sum_{n=1}^{\infty} \int \dots \int \frac{t(x_1) \dots t(x_n)}{n!} k_n(x_1, \dots, x_n) dx_1 \dots dx_n, \quad (7.48)$$

so that

$$\langle J[t] \rangle = e^{C[t]}. \quad (7.49)$$

We then immediately see that, for a “free” CQ field theory, the $n = 2$ cumulant in momentum space is the only one different from zero.⁶

One more generally finds

⁶ This ultimately follows from the following Gaussian integration: $\sqrt{\alpha/\pi} \int e^{\alpha x^2} e^{tx} dx = e^{t^2/4\alpha}$.

$$\begin{aligned}
\mu_1 &= k_1 \\
\mu_2 &= k_2 + k_1^2 \\
\mu_3 &= k_3 + 3k_1k_2 + k_1^3 \\
\mu_4 &= k_4 + 4k_3k_1 + 3k_2^2 + 6k_2k_1^2 + k_1^4 \\
&\dots = \dots
\end{aligned}$$

For a massive “free” field theory in CQ, the vacuum expectation value of the field is $\langle \varphi(x) \rangle = 0$. In $n = 4$ dimensions with $m = 1$, $N = 15$, $L = 3$, $a = L/N = 0.2$, we obtained in Ref. [6] the result shown in Fig. 7.1 where we compare the MC results with the exact expression of Eq. (7.46) with an infrared cutoff of $irc = 2$ which is sufficient for an accuracy of 10^{-3} . The run was $P = 10^6$ MC steps long. The figure shows good agreement between the MC and the exact expression except at the origin due to the spacetime discretization.

For a “free” $g \rightarrow 0$ massive theory in $n = 4$ dimensions with a self-potential energy $\frac{1}{2}m^2\varphi^2$ in AQ as in (7.1) but not regularized, the self-interaction is a double well with a spike barrier at $\varphi = 0$. In Fig. 7.2, we show the MC result for a “free” real scalar field subject to AQ with a total self-interaction of the form $V(\varphi) = \frac{1}{2}m^2\varphi^2 + \frac{3}{8}a^{-2s}/\varphi^2$ with $m = 1$, $N = 15$, $L = 3$, $a = L/N = 0.2$, after cutting the first equilibration MC steps of a run made of $P = 2.5 \times 10^6$ steps.

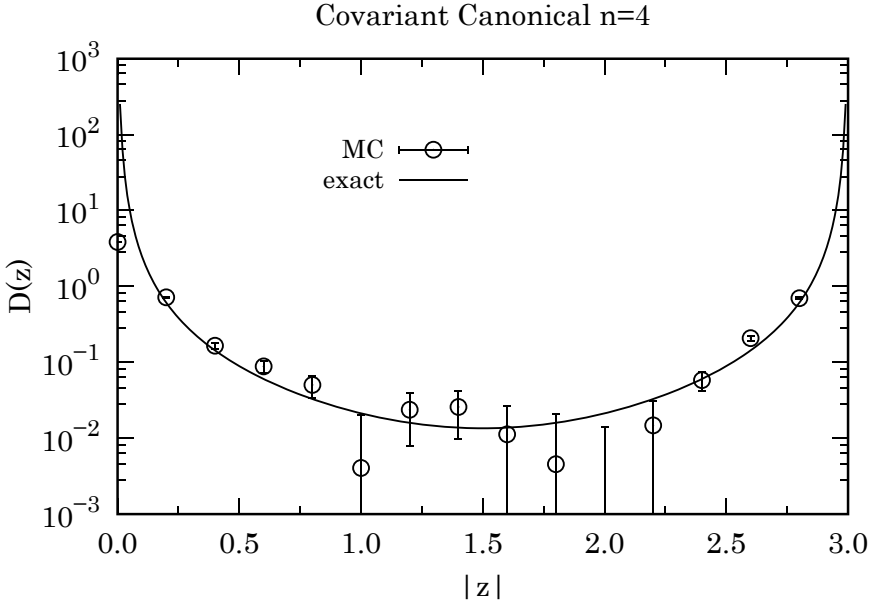


Fig. 7.1 Two-point connected function $D(z)$ of Eq. (7.43), for a free real scalar field subject to CQ in $n = 4$ dimensions with $m = 1$, $N = 15$, $L = 3$, $a = L/N = 0.2$. We compare with the analytic exact expression of Eq. (7.46) with an infrared cutoff of $irc = 2$. A logarithmic scale is used on the y-axis. This is Fig. 1 in Ref. [6]

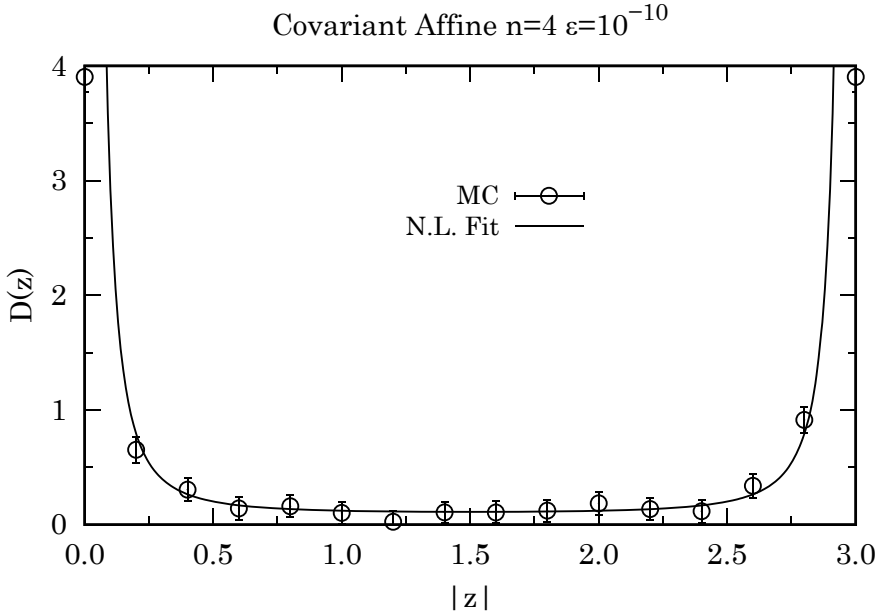


Fig. 7.2 Two-point connected function $D(z)$ of Eq. (7.43), for a free real scalar field subject to AQ in $n = 4$ dimensions as in Eq. (7.1) but not regularized, with $m = 1$, $N = 15$, $L = 3$, $a = L/N = 0.2$, and a random walk starting from an initial configuration with $\varphi(x) = \varepsilon = 10^{-10}$ for all x . Also shown is the result of a Non-linear Fit of the data (except the first point at $|z| = 0$) with the function $D_{m_D}(z)$ where D_{m_D} is the two-point function of a free field of mass m_D of Eq. (7.46) with an $irc = 2$, taking m_D as the only fit parameter

As we can see from the figure the symmetry $z \rightarrow L - z$ of the two-point function is preserved within the errorbars. The minima of the potential part of the classical action $\mathcal{V} = \sum_x V(\varphi(x))$ is at $\varphi = \pm\Phi$ with $\Phi = a^{-s/2} 3^{1/4} / \sqrt{2m}$ which diverges in the continuum limit $a \rightarrow 0$. Moreover the minimum of $\mathcal{V}$ is $L^{s+1} m \sqrt{3} / 2a^{2s+1}$ which also diverges, both in the continuum limit at finite volume ($ma \rightarrow 0$) and in the infinite volume limit at fixed lattice spacing ($mL \rightarrow \infty$).

The symmetry $\varphi \rightarrow -\varphi$ is broken in the simulations and as a result $\langle \varphi(x) \rangle$ is different from zero. Imagine now that we are in a configuration where all the N^n components, $\varphi(x)$, are around $+\Phi$. In order to start migrating one single x' component, $\varphi(x')$, around the other minimum at $-\Phi$ will have no cost in the potential, $\Delta\mathcal{V} \approx 0$, but it will have a big cost in the kinetic term between “neighboring” x , resulting in a big $\Delta\mathcal{K} \gg 0$ (as long as the distance between the two minima, 2Φ , which diverges in the continuum limit, is large). As a consequence $\exp(-\Delta\mathcal{S})$ will be very small and the move will be almost surely rejected according to the Metropolis rule. Moreover, once the system reaches the phase with all $\varphi(x)$ in one of the minima, it is very unlikely that a single $\varphi(x')$ will move to the other minimum but it cannot be excluded, in principle. If this happens one has a situation where the field is around $+\Phi$ at all x except at x' where it is around $-\Phi$. But we can easily see that

now it would be statistically favorable for the single field on the left to rejoin the fields on the right other than all the fields on the right join the field on the left. On the other hand, this would not hold for an *ultralocal* [17] theory where we could have the field visiting both wells at $\pm\Phi$ but only at not “neighboring” times, resulting in a vanishing $\langle\varphi(x)\rangle$. Apart from this the shape of the two-point function is qualitatively similar to the one of the *covariant* case. In addition in a covariant *complex* field one could go “slowly” “around” the “mountain” at $\varphi = 0$ with no need of “jumps”. This case has been studied in Ref. [7].

Due to the unphysical divergence of the vacuum expectation value of the field we found necessary to adopt the regularization through the scaling mentioned at the end of Sect. 6.2 and employed in Eq. (7.1). This allowed us to find for $V(\varphi)$ again a double well with a spike barrier at $\varphi = 0$ but now the separation of the two symmetric minima remains constant in the continuum $a \rightarrow 0$ limit.

In Ref. [18], we studied the continuum limit of the one- and two-point functions for the $(\varphi^4)_4$ AQ field theory which has the action of Eq. (7.1) for $n = r = 4$. What we see is that in this case the regularized case has a $V(\varphi) = \frac{1}{2}m^2\varphi^2 + g\varphi^r + \frac{3}{8}/\varphi^2$ which again shows a double well with a spike barrier at $\varphi = 0$ with symmetric minima at $\pm\Phi(m, g)$. In particular we find

$$\Phi(m, g) = \frac{3^{1/4}}{\sqrt{2m}} + O(m^{-7/2}) \quad \text{for } m \gg 1. \quad (7.50)$$

But in order for the finite-size effects to be negligible the bare Compton wavelength ($1/m$) must be small compared to the side (L) of the simulation box and at the same time, the lattice spacing (a) must be small compared to it. Namely

$$1/L \ll m \ll 1/a. \quad (7.51)$$

Therefore, next we considered the study case with $g = L = \beta = 1, m = \sqrt{N}/L$ with $a = L/N$ and allowing N to increase to approach the continuum limit. What we see in the simulation is that $\lim_{N \rightarrow \infty} \langle\varphi\rangle = \lim_{N \rightarrow \infty} \Phi(\sqrt{N}, 1) = 0$ in agreement with the results in Refs. [1–3, 5, 8, 10, 19]. Note that in all these works the constraint of keeping the renormalized mass m_R approximately constant at increasing values of N , discussed in the next section, was made possible only by choosing a bare mass m increasing with N at constant bare coupling constant g . The random walk during the simulation can now “tunnel” through the barrier and this results in a vanishing of the vacuum expectation value of the field $\langle\varphi(x)\rangle = 0$.⁷ Therefore restoring the $\varphi \rightarrow -\varphi$ symmetry. In this case since the path in $\varphi(x)$ visits both regions $\varphi > 0$ and $\varphi < 0$ it is formally more appropriate to substitute the numerical factor $\frac{3}{8}$ with

⁷ Note that this is only possible because in our numerical calculation on the computer we can never reach the continuum limit exactly. Clearly in the $a \rightarrow 0$ limit this “tunneling” would be forbidden due to the divergence of the kinetic term. This constitutes the very difference between affine canonical variables and Ashtekar canonical variables which, on the other hand, exclude only the single point at $\varphi = 0$.

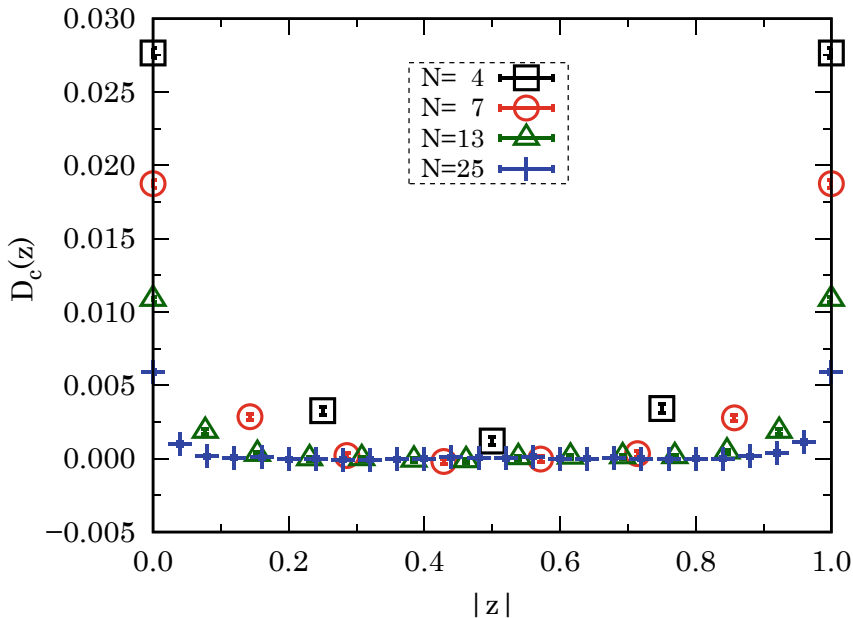


Fig. 7.3 Two-point connected function $D(z)$ for $n = 3 + 1$, $g = L = \beta = 1$, $m = \sqrt{N}/L$ and $N = L/a = 4, 7, 13, 25$. In our PIMC simulations, we used Eqs. (7.2) and (7.1)

1 in the potential energy term stemming from the AQ procedure, the last term in Eq. (7.1), following the results of Sect. 6.3.3.

From Fig. 7.3, we see the continuum limit $N \rightarrow \infty$, of the scaled two-point connected function $D(z)$. Respect to the work [6] (see Fig. 3 there) which dealt with the unscaled “free” field case and $D(0)$ was found to increase with increasing N we see how now the scaling has the effect of letting the value of $D(0)$ decrease with increasing N , as shown in Fig. 7.3, since $\varphi^{\text{scaled}} = \varphi^{\text{unscaled}}/N^{3/2}$ and $D^{\text{scaled}} = D^{\text{unscaled}}/N^3$. It is only tuning the bare mass m so to have a constant renormalized mass m_R for each N , that we would find true convergence. Unfortunately, this procedure is not easily accomplished numerically since for each N we would have to make several test runs with different values of m in order to find the value which keeps m_R approximately constant. This procedure was nonetheless carried out in the following works [1–3, 5, 8, 10, 19].

7.4 Triviality or Nontriviality

In this last section, I want to discuss the project that originally John proposed me and from which everything started⁸. That is the triviality of those CQ covariant

⁸ Much of the material of this section has been extracted from our Refs. [3, 10, 18].

Euclidean relativistic scalar field theories with a bare mass $m \geq 0$ and a bare coupling constant $g \geq 0$ with a potential self-interaction term such as $\varphi(x)^r$ with r a positive integer, in spacetime dimension $n = s + 1$, what we called a $(\varphi^r)_n$ theory, such that $r \geq 2n/(n - 2)$ (or $r > 2$ and any n for the corresponding ultralocal theory) that we already discussed in Sect. 6.1.1 (and Sect. 6.4 for the ultralocal case). The lattice version of these models can be shown to be trivial or become “free” in their continuum limit [1, 2, 5, 20].

In a sequel of recent papers [1–3, 5–10, 19], we proved, through path integral Monte Carlo (PIMC), that indeed AQ is able to make the $(\varphi^4)_4$ and $(\varphi^{12})_3$ theories nontrivial or “non-free” in their continuum limit.

The proposal of John, as soon as he realized that I was able to do MC, was to repeat the CQ calculation of Freedman et al. [21] but now for AQ. And see whether the problem of triviality would remain or would disappear. The idea of Freedman et al. is simple. Calculate, through PIMC, the renormalized coupling g_R of the given CQ field theory as a function of the bare coupling constant g at various increasing values of N being careful to fine tune the bare mass m so that, the corresponding value of m_R stays roughly constant as a function of g and N . This would in fact assure that we were studying a renormalized system where only the coupling constant was subject to vary with the mass being constant. Plotting then $g_R(g)$ one should be able to see whether g_R tends or not to zero increasing N , i.e., getting closer to the continuum $a \rightarrow 0$, for a given g . What Freedman et al. are able to show numerically is that while for the $(\varphi^4)_3$ theory $g_R(g)$ remains strictly positive for all N , for the $(\varphi^4)_4$ theory $g_R(g) \rightarrow 0$ at increasing values of N for all g . They therefore conclude that the φ^4 CQ covariant Euclidean relativistic scalar field theory is trivial in four spacetime dimensions but not in three.

Now the only delicate point in Freedman et al. numerical approach to the triviality problem is being able to choose the bare mass m so to keep the renormalized mass $m_R(m, g, N)$ constant as a function of g and N . This is so because, since we do not dispose of an analytic expression for m_R , there is no other way to do this than performing several brief test runs of the MC simulation at different close values of m . This can be very time consuming and is not guaranteed to give a precise way to find the proper values of m . And it represents the main source of uncontrolled uncertainty in their numerical approach.

In Figs. 7.4, 7.5, and 7.6 we show some of our PIMC results on the triviality problem for the $(\varphi^{12})_3$ and $(\varphi^4)_4$ covariant scalar field theories. In all these case studies we kept the renormalized mass $m_R \approx 3$ within 10%.

For our results on the triviality problem of the ultralocal $(\varphi^4)_2$ see Ref. [1]. In this case in the AQ theory the renormalized coupling constant does not seem to go toward zero at least when the bare coupling constant is zero when one approaches the continuum limit. Once again this means that scaled AQ theory is profoundly different from the “free” CQ one; the former is nontrivial and renormalizable and the latter is trivial and nonrenormalizable. For our results on the triviality problem of the restricted space field theory of Eq. (6.17) see Ref. [9]. Here we studied through PIMC a plausible kinetic factor in AQ of a scalar covariant Euclidean field theory of mass m subject to a potential energy of the form $g(\varphi^2 - \Phi^2)^2$ in $3 + 1$ spacetime dimensions,

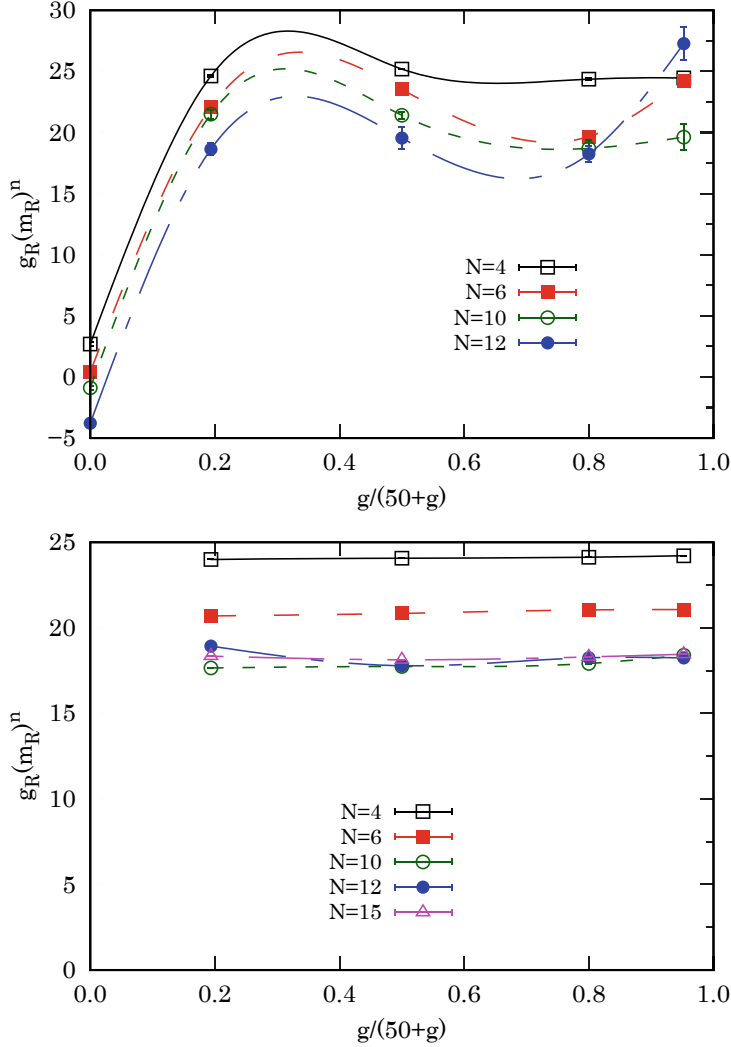


Fig. 7.4 We show the renormalized coupling constants $g_R(m_R)^n$ ($m_R \approx 3$) for various values of the bare coupling constant g at decreasing values of the lattice spacing $a = 1/N$ ($N \rightarrow \infty$ continuum limit) for the CQ (top panel) [5] and scaled AQ (bottom panel) [10] $(\varphi^{12})_3$ covariant Euclidean scalar field theory for $r = 12$, $n = 3$. Note that $g_{\text{top-panel}} = a^{5(n-1)} g_{\text{bottom-panel}}$ and for the action $S_{\text{top-panel}} = a^{n-1} S_{\text{bottom-panel}}$. The statistical errors were in all cases smaller than the symbols used. The main source of uncertainty is nonetheless the indirect one stemming from the unavoidable difficulty of keeping the renormalized mass constant throughout all cases [21]. The lines connecting the simulation points are just a guide for the eye

which is known to suffer from asymptotic freedom in the continuum limit when it is quantized through CQ. In fact such CQ model can be obtained from the φ_4^4 model introduced in Sect. 6.2 by changing $m^2 \rightarrow m^2 - 4g\Phi^2 \equiv M^2$ which will become negative for g big enough therefore producing a self-interaction potential with the

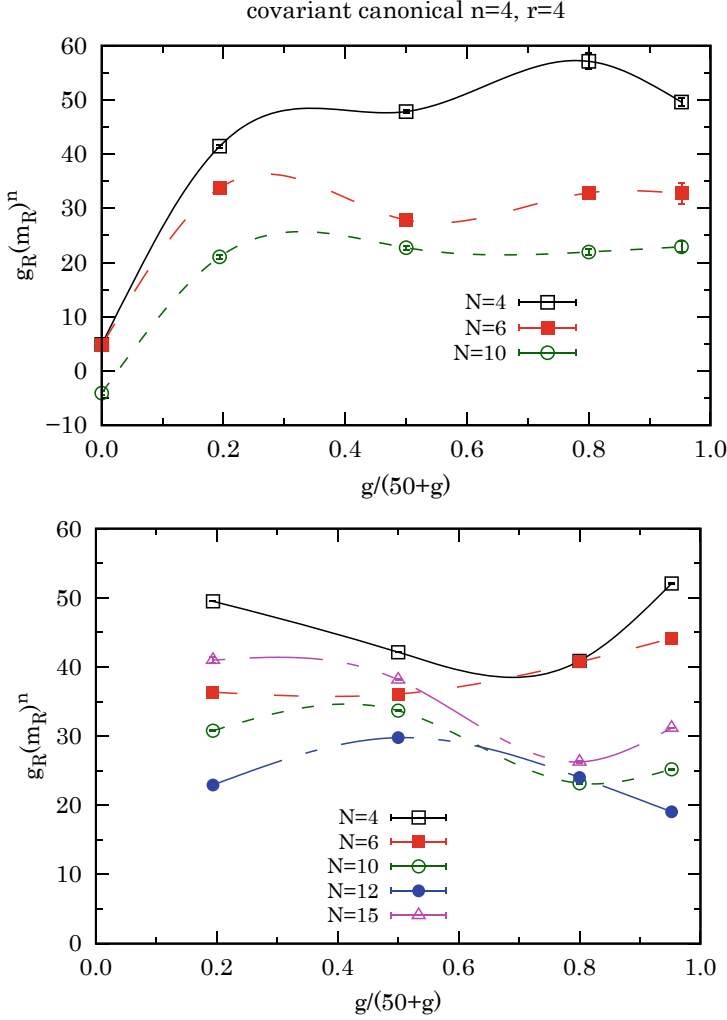


Fig. 7.5 We show the renormalized coupling constants $g_R(m_R)^n$ ($m_R \approx 3$) for various values of the bare coupling constant g at decreasing values of the lattice spacing $a = 1/N$ ($N \rightarrow \infty$ continuum limit) for the CQ (top panel) [2] and scaled AQ (bottom panel) [8] $(\varphi^4)_4$ covariant Euclidean scalar field theory for $r = 4$, $n = 4$. Note that $g_{\text{top-panel}} = a^{n-1} g_{\text{bottom-panel}}$ and for the action $S_{\text{top-panel}} = a^{n-1} S_{\text{bottom-panel}}$. The statistical errors were in all cases smaller than the symbols used. The main source of uncertainty is nonetheless the indirect one stemming from the unavoidable difficulty of keeping the renormalized mass constant throughout all cases [21]. The lines connecting the simulation points are just a guide for the eye

profile of a symmetric double well with the two minima, at $\varphi_{\pm} = \pm \sqrt{-M^2/4g}$. The AQ kinetic factor in this case reduces to the usual one previously introduced in the limit $\Phi \rightarrow 0$, apart from the multiplicative coefficient change $3/4 \rightarrow 2$. Moreover its behavior is similar to the one found in the $\Phi \rightarrow 0$ limit in the sense that it gives

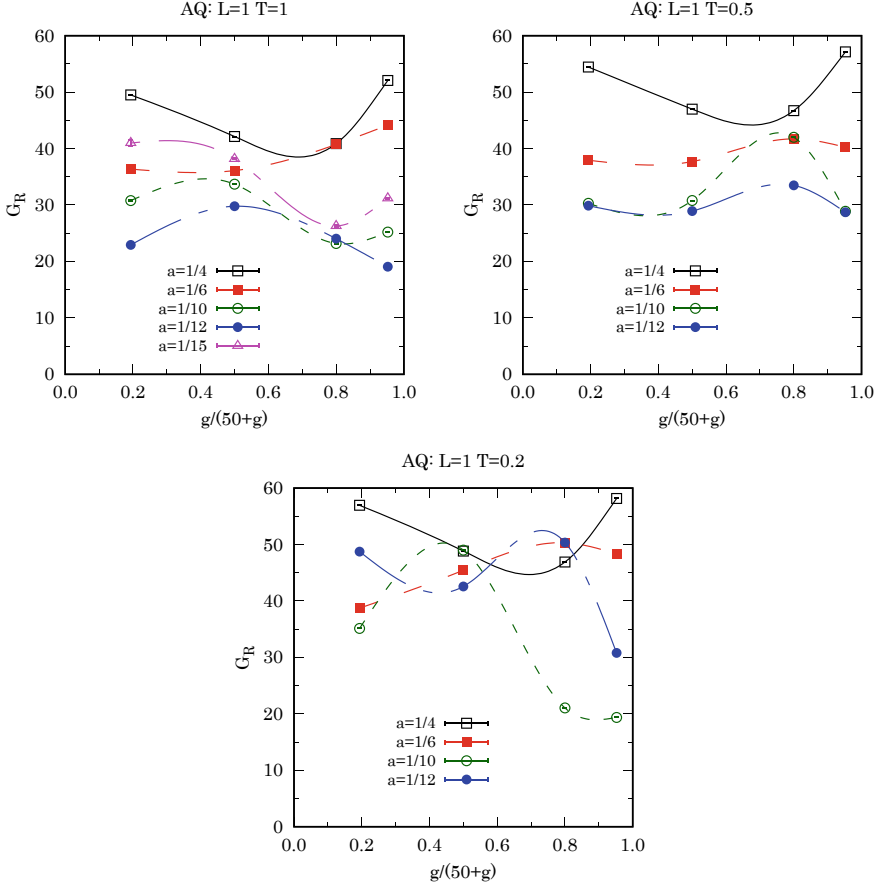


Fig. 7.6 We show the low temperature behavior for the $(\varphi^4)_4$ theory [3]. The top left panel is for scaled AQ with the box side $L = 1$ and the absolute temperature $T = 1$, the top right panel is for scaled AQ with $L = 1$ and $T = 0.5$, and the bottom panel is for scaled AQ with $L = 1$ and $T = 0.2$. We show the renormalized coupling constant $G_R = g_R(m_R)^n/T$ as a function of $g/(50 + g)$ for decreasing values of the lattice spacing $a = L/N$. The renormalized mass was kept fixed to $m_R \approx 3$ (within 10%) in all cases. The statistical errors in the Monte Carlo were in all cases smaller than the symbols used. The main source of uncertainty is nonetheless the indirect one stemming from the unavoidable difficulty of keeping the renormalized mass constant throughout all cases [21]. The lines connecting the points are just a guide for the eye

rise to an additive effective self-interaction potential term which diverges at $\varphi = \pm\Phi$ (see Eq. 6.18) in a neighborhood of the minima $\varphi_{\pm}$, therefore producing a forbidden region for the field paths exactly where it would naturally sit in a CQ framework. This exclusion of the field path from the minima of the potential renders the AQ version of the field theory asymptotically “non-free” in the continuum limit. Our numerical results clearly show how the two field theories obtained through CQ and AQ behave very differently whenever $m^2/4g \ll \Phi^2$. Otherwise they are very similar.

All these numerical results suggest that using AQ cures, in all studied field theory cases, the triviality otherwise observed in the corresponding CQ version. We found these results very encouraging and even if not a complete mathematical proof of the nontriviality they yet constitutes a strong indication in its favor. Remember that a MC simulation is just an exact (up to the statistical uncertainties and the finite-size effects) numerical solution of a multidimensional integral, so that our results are still valuable for the given lattice field theory. Of course the approach to the continuum limit was limited by the computational resources that have not been extraordinary since we did not have any source of funding during our collaboration, and they were much more severe as spacetime dimensions were chosen to increase. Moreover, for me, coming from the many-body physics community, it has been a pleasure to discover that the simulation of a quantum field theory (through path integral techniques) is actually just a *single particle* problem, so much simpler than the kind of problems I was accustomed to deal with!

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Chapter 8

Complex Scalar Field Theory



*Poi fummo dentro al soglio de la porta
che 'l mal amor de l'anime disusa,
perchè fa parer dritta la via torta,*

*Dante Alighieri
La Divina Commedia (canto X purgatorio)*

Abstract In this chapter, we present the quantum relativistic Euclidean complex scalar field theory describing the Higgs Mexican-hat system as treated through Canonical and Affine Quantization, the scaling regularization necessary in Affine Quantization is discussed, and the numerical results from our Path Integral Monte Carlo Numerical Experiments are discussed.

The aim of this chapter¹ is to find out what affine quantization [2, 3] does to a classical field theory for two real scalar fields, or equivalently a complex scalar field, of mass m subject to the Mexican-hat, Higgs potential, rather than canonical quantization [4]. To this aim, we will compare the two-point function of the two fields in the two frameworks.

In particular, here we try to understand in what ways an affine quantization is similar as well as dissimilar from a canonical quantization. We add that some non-free real scalar fields have already been observed and that canonical quantization fails for several nonrenormalizable fields, such as $(\phi^{12})_3$ [5] and $(\phi^4)_4$ [6]. The key to that result is the introduction of a highly unusual, additional, non-quadratic, term that is dictated by affine quantization. While affine quantization employs an additional term, that particular term formally disappears when the Planck constant $\hbar \rightarrow 0$, which makes it a plausible modification of the quadratic terms of traditional free real scalar fields in order to extend acceptable quantization of traditional nonrenormalizable models [7–10].

¹ Much of its material is extracted from our Ref. [1].

This should be considered as a follow up of our previous work [11] where the two-point function of a single Euclidean free real scalar field subject to affine quantization was found through Monte Carlo (MC) methods. In particular, in that work, we found that the vacuum expectation value of the field diverges in the continuum limit. This shortcoming is expected to disappear in the present case of a complex field $\varphi = \phi_1 + i\phi_2$. In fact, in this case, one can go “slowly” “around” the peak at $\varphi = 0$ with no need of “jumps” [11].

The covariant Euclidean action in canonical quantization [4] is²

$$S^{(c)}[\phi_1, \phi_2] = \int \left\{ \frac{1}{2} \sum_{\mu=0}^s \left[\left(\frac{\partial \phi_1(x)}{\partial x_\mu} \right)^2 + \left(\frac{\partial \phi_2(x)}{\partial x_\mu} \right)^2 \right] + V(\phi_1(x), \phi_2(x)) \right\} d^n x, \quad (8.1)$$

$$V(\phi_1, \phi_2) = \frac{1}{2} m^2 (\phi_1^2 + \phi_2^2) + g [(\phi_1^2 + \phi_2^2) - \Phi^2]^2, \quad (8.2)$$

with $x = (x_0, x_1, \dots, x_s) = (x_0, \mathbf{x})$ for s spatial dimensions and $n = s + 1$ for the number of spacetime dimensions with $x_0 = ct$, where c is the speed of light constant and t extends from zero to $\hbar\beta$ with $\beta = 1/k_B T$, k_B being the Boltzmann constant and T the absolute temperature. We will work at $s = 3$. And V is the self-interaction potential density corresponding to an interacting Higgs theory with a bare mass m and a bare coupling g .

The covariant Euclidean action in affine quantization [2, 3] is

$$S^{(a)}[\phi_1, \phi_2] = \int \left\{ \frac{1}{2} \sum_{\mu=0}^s \left[\left(\frac{\partial \phi_1(x)}{\partial x_\mu} \right)^2 + \left(\frac{\partial \phi_2(x)}{\partial x_\mu} \right)^2 \right] + \frac{3}{8} \frac{\delta^{2s}(0) \hbar^2}{\phi_1^2(x) + \phi_2^2(x)} + V(\phi_1(x), \phi_2(x)) \right\} d^n x, \quad (8.3)$$

where the “3/8” extra term stems from considering the complex field $\varphi(x) = \phi_1(x) + i\phi_2(x)$ and the momentum field $\pi(x) = -i\hbar\partial/\partial\varphi(x)$ as the two conjugate canonical variables (see Appendix A in [5]) and δ is a Dirac delta function. In this case, the Hamiltonian density formally contains a divergent term in the total potential density $\mathcal{V}(\phi) = \frac{3}{8}\delta^{2s}(0)\hbar^2/(\phi_1^2 + \phi_2^2) + V(\phi)$, in the continuum, but the field theory can be regularized and treated on a lattice, and the *approach* toward the continuum will be taken under exam in this work. In the following, we will use natural units with $c = \hbar = k_B = 1$.

In our previous works, we studied the single real scalar field nonrenormalizable canonical cases with $V(\phi) = \frac{1}{2}m^2\phi^2 + g\phi^4$ [6] in $s = 3$ and $\frac{1}{2}m^2\phi^2 + g\phi^{12}$ in $s = 2$ [5], where g is the bare coupling constant. And we showed that the corresponding affine cases are indeed renormalizable.

² Note however that Eq. (8.2) can be simplified to $V = g[(\phi_1^2 + \phi_2^2) - A^2]^2 + \text{constant}$, where A involves a combination of Φ and m : $A^2 = \Phi^2 - m^2/4g$.

MC [12, 13] is the numerical method of choice to treat multidimensional integrals of high dimensions and, therefore, is especially useful to compute path integrals. We will use it to study the two-point function of the Euclidean action of two real scalar field in affine quantization. Our estimate of the path integrals will be generally subject to three sources of numerical uncertainties: The one due to the statistical errors, the one due to the spacetime discretization, and the one due to the finite-size effects. Of these, the statistical errors scale like $M^{-1/2}$ where M is the computer time, the discretization of spacetime is responsible for the distance from the *continuum limit* (which corresponds to a lattice spacing $a \rightarrow 0$), and the finite-size effects stems from the necessity to approximate the infinite space system with one in a periodic box of volume L^s with $L = Na$ being the box side, subject to N discretization points. The finite-size effects are due to the distance from the *thermodynamic limit* (which corresponds to $N \rightarrow \infty$) [14].

8.1 The Lattice Formulation of the Field Theory Model

We used a lattice formulation of the field theory. The theory considers a complex scalar field $\varphi = \phi_1 + i\phi_2$ taking the value $\varphi(x)$ on each site of a periodic, hypercubic, n -dimensional lattice of lattice spacing a and periodicity $L = Na$. The canonical covariant action for the field, Eq. (8.1), is then approximated by

$$\begin{aligned} \frac{S^{(c)}[\phi_1, \phi_2]}{a^n} \approx \frac{1}{2a^2} \sum_{x, \mu} \left\{ [\phi_1(x) - \phi_1(x + e_\mu)]^2 + [\phi_2(x) - \phi_2(x + e_\mu)]^2 \right\} + \\ \sum_x V(\phi_1(x), \phi_2(x)), \end{aligned} \quad (8.4)$$

where e_μ is a vector of length a in the $+\mu$ direction and we are at a temperature $T = 1/Na$, in units where Boltzmann constant $k_B = 1$.

Note that in our model the continuous symmetry $\varphi \rightarrow e^{i\alpha}\varphi$ breaks down spontaneously and the mass spectrum contains a Goldstone boson. The accepted signal of a system being in the symmetry broken phase in a finite volume, in the absence of a small symmetry breaking term, is not a non-zero-order parameter, but rather the fact that a product of order parameters, at points x, y , tends to a non-zero limit with increasing $|x - y|$. To understand the properties of the system at finite volume, it is convenient to add a small symmetry breaking term and to with the potential

$$V = g(\phi_1^2 + \phi_2^2 - A^2)^2 + (\epsilon^2/2)\phi_2^2 + \text{constant}, \quad (8.5)$$

The term proportional to ϵ^2 ensures that the classical action has a proper minimum at the point $\phi_1 = A, \phi_2 = 0$. The expansion of the potential in powers of $\psi = \phi_1 - A$, and ϕ_2 starts with

$$V = (M^2/2)\psi^2 + (\varepsilon^2/2)\phi_2^2 + \dots, \quad (8.6)$$

$$M = A\sqrt{8g}. \quad (8.7)$$

The first term represents a free particle of mass M , the second a free particle of mass ε . The situation is the same as in the case of the free real scalar field: the perturbative expansion of the two-point function starts with

$$\langle \phi_1(x)\phi_1(y) \rangle = A^2 + D(x-y, M, L), \quad (8.8)$$

$$\langle \phi_2(x)\phi_2(y) \rangle = D(x-y, \varepsilon, L), \quad (8.9)$$

$$\langle \phi_1(x)\phi_2(y) \rangle = 0, \quad (8.10)$$

where $\langle \dots \rangle$ is the vacuum expectation value (defined in Eq. (8.14)) and $D(z, m, L)$ is the propagator of a free particle of mass m on a hypercubic Euclidean box of size L^n . For $\varepsilon = 0$, the term $D(z, \varepsilon, L)$ reduces to a sum of free massless propagators:

$$D(z, 0, L) = (1/4\pi^2) \sum_{n_0, n_1, n_2, n_3} 1/[(z_0 + n_0L)^2 + \dots + (z_3 + n_3L)^2], \quad (8.11)$$

where $z = (z_0, z_1, \dots, z_s)$ and $n_\mu \in \mathbb{Z}$ for $\mu = 0, 1, \dots, s$, but this expression does not make sense because the sum diverges. As long as ε is different from zero, the limit $L \rightarrow \infty$ ensures that a single term in the sum survives, the one with $n_0 = \dots = n_3 = 0$, which describes the contribution from the Goldstone boson.

Expression (8.4) needs to be modified for the affine action of Eq. (8.3). In this case, the Dirac delta function is replaced by $\delta^{2s}(0) \rightarrow a^{-2s}$. Moreover, it is convenient the following scaling: $\phi_i = a^{-s/2}\bar{\phi}_i$, and $\Phi_i = a^{-s/2}\bar{\Phi}_i$, $g = a^s\bar{g}$ which gives the following discretized approximation for the affine action:

$$\begin{aligned} \frac{S^{(a)}[\bar{\phi}_1, \bar{\phi}_2]}{a^{-s}a^n} &\approx \frac{1}{2a^2} \sum_{x, \mu} \left\{ [\bar{\phi}_1(x) - \bar{\phi}_1(x + e_\mu)]^2 + [\bar{\phi}_2(x) - \bar{\phi}_2(x + e_\mu)]^2 \right\} + \\ &\sum_x \frac{3}{8} \frac{1}{\bar{\phi}_1^2(x) + \bar{\phi}_2^2(x)} + \\ &\sum_x \left\{ \frac{1}{2} m^2 (\bar{\phi}_1^2(x) + \bar{\phi}_2^2(x)) + \bar{g} [(\bar{\phi}_1^2(x) + \bar{\phi}_2^2(x)) - \bar{\Phi}^2]^2 \right\}. \end{aligned} \quad (8.12)$$

Note that if g is taken different from zero, the relation $g = a^s\bar{g}$ shows that $\bar{g}$ carries a dimension. Setting $\bar{g} = M^s$, M is of dimension mass (we are using natural units $c = \hbar = 1$). If M as well as m are kept fixed when the cutoff is removed, the model contains the two dimension-full parameters m and M . The lattice spacing a must be small compared to $1/m$ as well as compared to $1/M$ and the box must be large compared to $1/M$. Since $\bar{\phi}$ is of dimension $\text{mass}^{-1/2}$, the two-point function of $\bar{\phi}$ is of the form

$$\langle \bar{\phi}_i(x)\bar{\phi}_j(y) \rangle = f_{ij}\{M(x-y), m/M, aM, LM\}/M. \quad (8.13)$$

To approach the continuum limit, the last two argument must be in the range: $aM \ll 1$, $LM \ll 1$. The only relevant parameter, apart from the number of lattice points, used to regularize the system should be the ratio m/M .

We will use the so-called “primitive approximation” for the action (see Eqs. (8.4) or (8.12)) even if it can be improved in several ways [15] in order to reduce the error due to the spacetime discretization. In reaching to the expression (8.4) or (8.12), we neglected the term $\propto a^{2n}$ due to the commutator of the kinetic and potential parts of the Hamiltonian, in the Baker–Campbell–Hausdorff formula. In reaching to the path integral expression this is justified by the Trotter formula.

The vacuum expectation of a functional observable $\mathcal{O}[\phi_1, \phi_2]$ is

$$\langle \mathcal{O} \rangle \approx \frac{\int \mathcal{O}[\phi_1, \phi_2] \exp(-S[\phi_1, \phi_2]) \prod_x d\phi_1(x) d\phi_2(x)}{\int \exp(-S[\phi_1, \phi_2]) \prod_x d\phi_1(x) d\phi_2(x)}, \quad (8.14)$$

for a given action S .

We will approach the continuum limit by choosing a fixed L and increasing the number of discretizations N of each component of the spacetime. So that the lattice spacing $a = L/N \rightarrow 0$. To make contact with the continuum limit, two conditions must be met $a \ll 1/m \ll L$ where $1/m$ is the Compton wavelength.

8.2 Simulation Details and Relevant Observables

We want to determine the two-point function

$$K_{ij}(x, y) = \langle \phi_i(x) \phi_j(y) \rangle, \quad (8.15)$$

where, in the affine case, we need to replace the fields ϕ_i by the scaled fields $\tilde{\phi}_i$. Replacing x by $x + k$ with $k = aw_n$ with $w_n = (n_0, n_1, \dots, n_s)$ and $n_\mu \in \mathbb{Z}$ amounts to a mere relabeling of the lattice points. Hence, due to translational invariance, $K(x, y)$ can only depend on the difference between the coordinates of the two points and we can define,

$$D_{ij}(z) = \frac{1}{L^n} \sum_x K_{ij}(x, x + z) a^n. \quad (8.16)$$

Moreover, due to the symmetry $1 \leftrightarrow 2$, we will have $D_{11} = D_{22} \equiv D_{\text{like}}$ and $D_{12} = D_{21} \equiv D_{\text{unlike}}$. In our simulations we work in periodic spacetime (at a temperature $T = 1/Na$) so that $\phi_i(x_\mu + N) = \phi_i(x_\mu)$ for any x , $\mu = 0, 1, \dots, s$, and $i = 1, 2$.

Our MC simulations use the Metropolis algorithm [12, 13] to calculate the ensemble average of Eq. (8.14) which is a $2N^n$ multidimensional integral. The simulation is started from the initial condition $\phi_i = \epsilon = 10^{-10}$ for $i = 1, 2$. One MC step con-

sisted in a random displacement of each one of the $2N^n$ variables $\phi_i(x)$ for $i = 1, 2$, as follows:

$$\phi_i \rightarrow \phi_i + (2\eta - 1)\delta, \quad (8.17)$$

where η is a uniform pseudo-random number in $[0, 1]$ and δ is the amplitude of the displacement. The fields $\phi_i \in (-\infty, \infty)$ for $i = 1, 2$ and $x_\mu \in [0, L]$ for $\mu = 0, 1, \dots, s$. Each one of these $2N^n$ moves is accepted if $\exp(-\Delta S) > \eta$ where ΔS is the change in the action due to the move (it can be efficiently calculated considering how the kinetic part and the potential part change by the displacement of a single $\phi_i(x)$) and rejected otherwise. The amplitude δ is chosen in such a way to have acceptance ratios as close as possible to $1/2$ and is kept constant during the evolution of the simulation. One simulation consisted of M MC steps each of which consisted in a sweep of $2N^n$ displacement moves of all the fields variables. The statistical error on the average $\langle \mathcal{O} \rangle$ will then depend on the correlation time necessary to decorrelate the property $\mathcal{O}$, $\tau_{\mathcal{O}}$, and will be determined as $\sqrt{\tau_{\mathcal{O}}\sigma_{\mathcal{O}}^2/(M2N^n)}$, where $\sigma_{\mathcal{O}}^2$ is the intrinsic variance for $\mathcal{O}$.

8.3 Simulation Results

We worked in natural units where $c = \hbar = k_B = 1$. In Fig. 8.1, we show $D_{\text{like}}(z)$ and $D_{\text{unlike}}(z)$ as obtained for $m = 1$, $g = 1$, $\Phi = 1$, $L = 3$ and three choices of N , in the canonical scenario. One can then see the approach to the continuum of the two-point functions of the canonical model. From the figure, we can see that the unlike two-point function is zero over the whole spacetime volume. This can be explained observing that during the random walk the field will be localized around the minima of the potential density so that $\phi_1^2 + \phi_2^2 \approx \Pi_c^2$ with Π_c the radius of the minima ring, the circle of vacua, around the origin $\varphi = 0$, which is a function of m , g and Φ :

$$\Pi_c^2 = \frac{4g\Phi^2 - m^2}{4g}. \quad (8.18)$$

So that the Higgs potential density in the action does not actually contribute to correlate the two fields ϕ_i for $i = 1, 2$. Moreover, the expectation values $\langle \phi_i \rangle = 0$ for $i = 1, 2$ because the complex field φ tends to rotate around the origin on the minima ring. The approach to the continuum is manifested through increasing values of $D_{\text{like}}(0)$ with increasing N . For our choice of the parameters $m^2 < 4g\Phi^2$ and we must have symmetry breaking [8–10], with the circle of vacua having a radius different from zero. The renormalized coupling constant [6] was found to be: $g_R = -0.0069(6)$ for $N = 8$, $g_R = -0.0006(4)$ for $N = 10$, $g_R = +0.0000(5)$ for $N = 13$. Since g_R must be non-negative, by Lebowitz inequality, our results signal a free trivial system in the continuum limit.

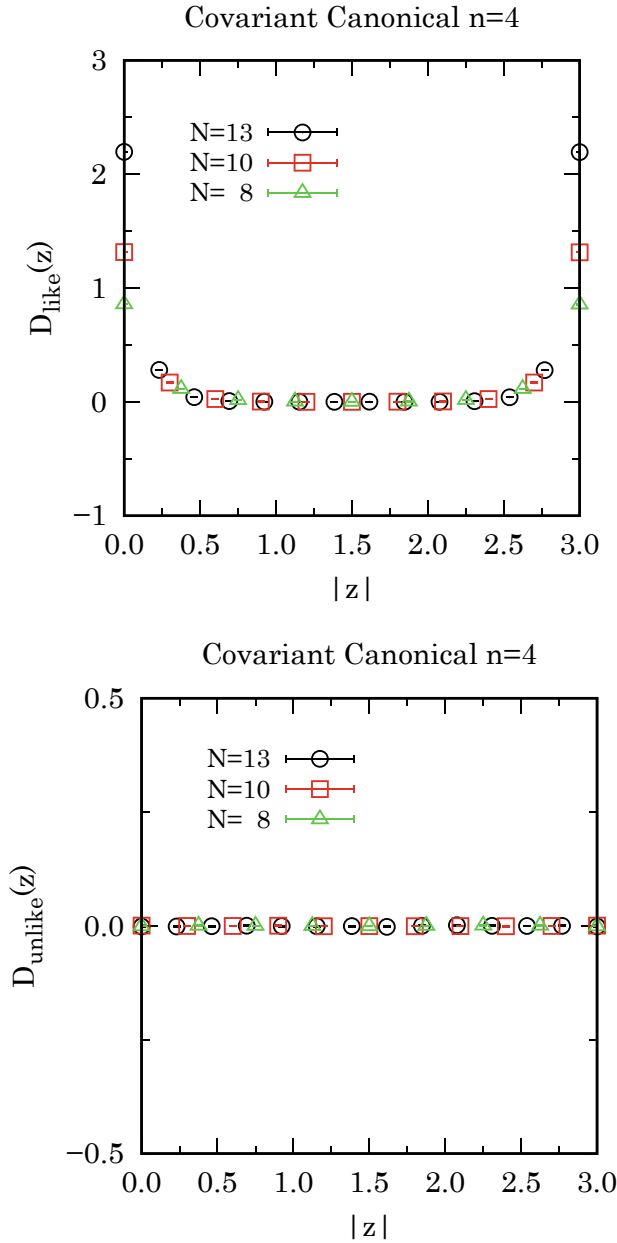


Fig. 8.1 (color online) Two-point functions, $D_{\text{like}}(z)$ (top panel) and $D_{\text{unlike}}(z)$ (bottom panel), of Eq. (8.16) for the complex scalar Higgs field $\varphi = \phi_1 + i\phi_2$ subject to canonical quantization with a self-interaction potential density of the form $V(\phi) = \frac{1}{2}m^2(\phi_1^2 + \phi_2^2) + g(\phi_1^2 + \phi_2^2 - \Phi^2)^2$ in Eq. (8.3) with $m = 1$, $g = 1$, $\Phi = 1$, $L = 3$ ($\Pi_c^2 = 3/4$) and increasing $N = 8, 10, 13$. On the abscissa axis, we have $|z| = \sqrt{z_0^2 + z_1^2 + \dots + z_s^2}$ which is a length

For the affine quantization case, the circle of vacua has a radius $\bar{\Pi}_a$, which is now a function of m , $\bar{g}$, and $\bar{\Phi}$:

$$\bar{\Pi}_a^2 = \frac{4\bar{g}\bar{\Phi}^2 - m^2}{12\bar{g}} + \frac{(4\bar{g}\bar{\Phi}^2 - m^2)^2}{12\bar{g}[162\bar{g}^2 + \Xi + 18\bar{g}^{2/3}(81\bar{g}^2 + \Xi)^{1/3}] + \frac{162\bar{g}^2 + \Xi + 18\bar{g}^{2/3}[81\bar{g}^2 + \Xi]^{1/3}}{12\bar{g}}}, \quad (8.19)$$

$$\Xi = -m^6 + 12\bar{g}m^4\bar{\Phi}^2 - 48\bar{g}^2m^2\bar{\Phi}^4 + 64\bar{g}^3\bar{\Phi}^6. \quad (8.20)$$

This is different from zero irrespectively from the values of the parameters, so symmetry is always broken. In Fig. 8.2, we show $D_{\text{like}}(z)$ and $D_{\text{unlike}}(z)$ as obtained for $m = 1$, $\bar{g} = 1$, $\bar{\Phi} = 1$, $L = 3$ (so that $m/M = 1$), and three choices of N , in the affine scenario, for the $\bar{\phi}_i$ fields introduced in Eq. (8.12). One can then see the approach to the continuum of the two-point functions of the affine model. Note, however, that now the region around $\bar{\phi}_i = 0$ for $i = 1, 2$ is forbidden due to the affine $3/8$ diverging term in the potential density (see Eq. (8.12)), therefore the complex field in its “winding” around the origin, in proximity of the potential minima ring, cannot take a “shortcut” through the “mountain” at the origin (the forbidden region) and this, in turn, is responsible for a loss of ergodicity and the appearance of systematic errors in addition to the usual statistical ones. It is then necessary an extremely long simulation (much longer than the average time for a “round trip” of the field), much longer than in the canonical case. Notice, moreover, that the action is penalized by the additional a^{-s} factor which grows as we approach the continuum $a \rightarrow 0$. A possible solution would be to choose the field displacement δ larger than the diameter of the potential minima ring $2\bar{\Pi}_a$. But unfortunately this will not work because the kinetic energy term in the action doesn’t allow the field to undergo big “jumps”. In addition this would generate low acceptance ratios thereby slowing down the simulation. An alternative solution will be given in the next section. In our simulations, that were $M = 10^7$ MC steps long, the expectation value of the field $\langle \bar{\phi}_1 \rangle = \langle \bar{\phi}_2 \rangle$ was equal to $-0.23(4)$ for $N = 8$, to $-0.24(4)$ for $N = 10$, and to $-0.784(9)$ for $N = 13$. A non-zero value for the vacuum expectation of the field is due to the systematic errors described above and will eventually disappear in an extremely long simulation. From the figure we see how the two-point like function seems to be increasing with N , while the unlike one has a constant behavior fluctuating around the expected zero value. These results are still affected by the ergodicity systematic errors stemming from the “winding” random walk. In order to show this behavior, we calculated the histograms of the values for $\langle \bar{\phi}_1 \rangle$ obtained by averaging over blocks of 100 MC steps during the simulation, that we call $H\bar{\phi}$, of $D_{\text{like}}(0)$ that we call $H D_{\text{like}}$, and of $D_{\text{unlike}}(0)$, that we call $H D_{\text{unlike}}$. The behavior of these histograms is shown in Figs. 8.3, 8.4, and 8.5 respectively. From the histogram

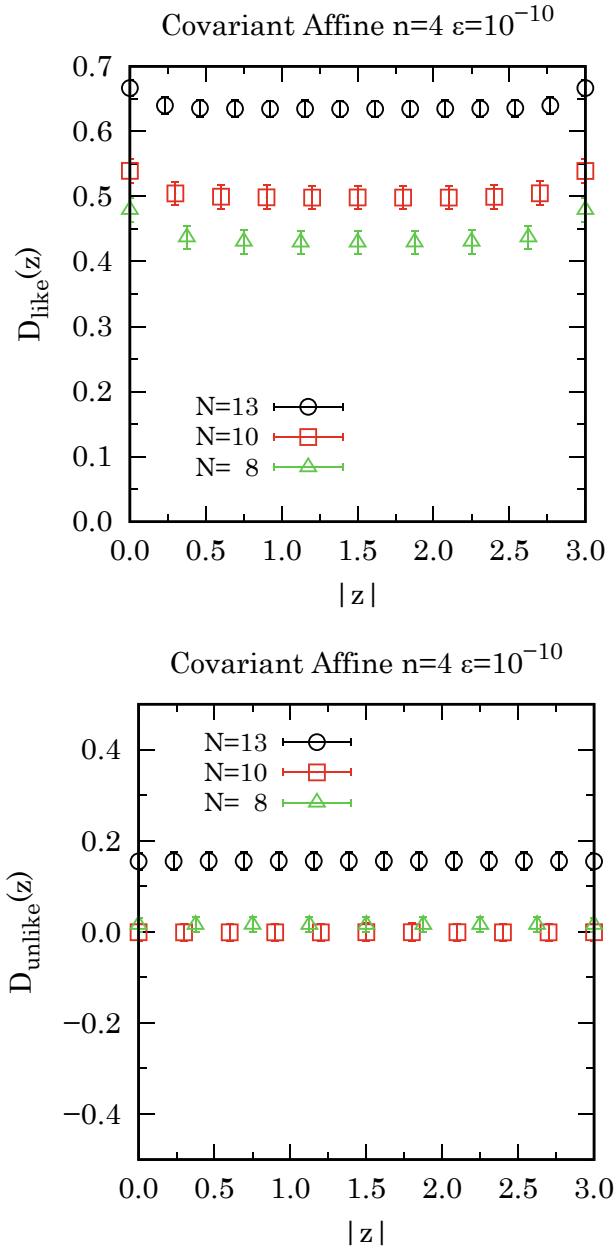


Fig. 8.2 (color online) Two-point functions, $D_{\text{like}}(z)$ (top panel) and $D_{\text{unlike}}(z)$ (bottom panel), of Eq. (8.16) for the complex scalar Higgs field $\bar{\varphi} = \phi_1 + i\phi_2$ subject to affine quantization with a self-interaction potential density of the form $V = \frac{1}{2}m^2(\bar{\phi}_1^2 + \bar{\phi}_2^2) + g(\bar{\phi}_1^2 + \bar{\phi}_2^2 - \bar{\Phi}^2)^2$ in Eq. (8.3) with $m = 1$, $\bar{g} = 1$, $\bar{\Phi} = 1$, $L = 3$ ($\bar{\Gamma}_a^2 \approx 0.955410$) in Eq. (8.12) and increasing $N = 8, 10, 13$. The simulation used $M = 10^7$ MC steps and started from the initial condition $\phi_i = \epsilon = 10^{-10}$ for $i = 1, 2$. On the abscissa axis we have $|z| = \sqrt{z_0^2 + z_1^2 + \dots + z_s^2}$ which is a length

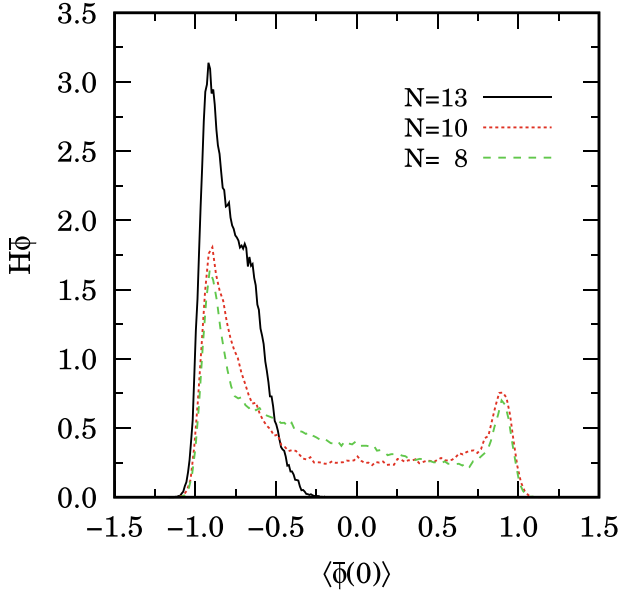


Fig. 8.3 (color online) Histogram of $\langle \bar{\phi}_1 \rangle$ block values during the simulation shown in Fig. 8.2. The figure shows the “rotation” of the field around the origin in proximity of the potential minima ring of radius $\bar{\Gamma}_a \approx 0.977451$, for $N = 8$ and 10 , but not for $N = 13$. Even for $N = 8$ and 10 the rotation was not symmetric (this would only be obtained in an extremely long simulation), which explains the not exactly zero value of the expectation value of field

of Fig. 8.3 we see how for $N = 13$ the field did not have the chance of rotating around the origin and this explains the lack of the first peak in the histogram of Fig. 8.4. We then conclude that the simulation for $N = 13$ was not long enough. And this is responsible for the high value of the two-point like function observed for $N = 13$, as shown in Fig. 8.2. In order to obtain a fully symmetric rotation of the field random walk around the origin we would clearly need an extremely long simulation. Nonetheless from the partial results of our long simulation we can gather a flavor of the convergence of the two-point functions in the affine case in the continuum limit at finite volume.

These results, albeit partial in their nature, give to affine quantization a role as a method producing meaningful quantum field theories even when, as we have already seen in our previous works [5, 6, 11], the more common canonical quantization fails. Moreover with the scaling used in Eq. (8.12) the field theory doesn’t suffer from the unpleasant feature of a diverging vacuum expectation value of the field in the continuum limit, which was observed in Ref. [11].

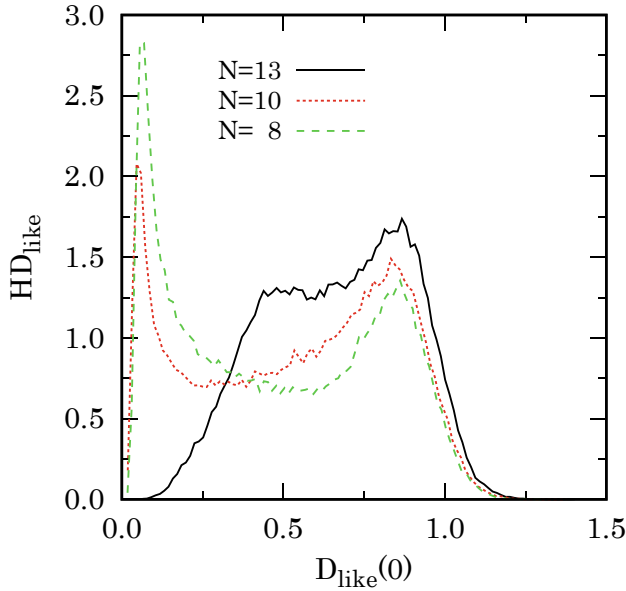


Fig. 8.4 (color online) Histogram of $D_{\text{like}}(0)$ block values during the simulation shown in Fig. 8.2. The missing first peak in the $N = 13$ data is due to the fact that the field didn't perform a full rotation around the origin as is shown by Fig. 8.3

8.4 Exponential Representation of the Complex Scalar Field

In order to solve the ergodicity breakdown problem encountered in the previous section for the affine case we decided to rewrite our path integral in terms of the fields $\rho(x)$ and $\theta(x)$ such that $\tilde{\varphi}(x) = \rho(x) \exp[i\theta(x)]$. Equation (8.12) may be rewritten as follows

$$\frac{S^{(a)}[\rho, \theta]}{a^{-s} a^n} \approx \frac{1}{2a^2} \sum_{x, \mu} \left\{ [\rho(x) - \rho(x + e_\mu)]^2 + \rho^2(x) [\theta(x) - \theta(x + e_\mu)]^2 \right\} + \sum_x \left\{ \frac{3}{8} \frac{1}{\rho^2(x)} + \frac{1}{2} m^2 \rho^2(x) + \bar{g} [\rho^2(x) - \bar{\Phi}^2]^2 \right\}, \quad (8.21)$$

and the path integral over $\rho \in [0, \infty]$ and $\theta \in [-\infty, \infty]$ will not suffer anymore from the ergodicity problem. In the Metropolis algorithm we will now have acceptance when $\exp[-(S' - S)] \prod_x \rho'(x)/\rho(x) > \eta$ where the primed quantities are the newly generated ones and as usual η is a pseudo random number in $[0, 1]$. The modulus displacement move, $\rho \rightarrow \rho' = \rho + (2\eta - 1)\delta_\rho$, is rejected whenever $\rho' < 0$. And the argument displacement move is chosen purposely asymmetric, $\theta \rightarrow \theta' = \theta + \eta\delta_\theta$, in order to allow for the required rotation and break the symmetry. This transition rule

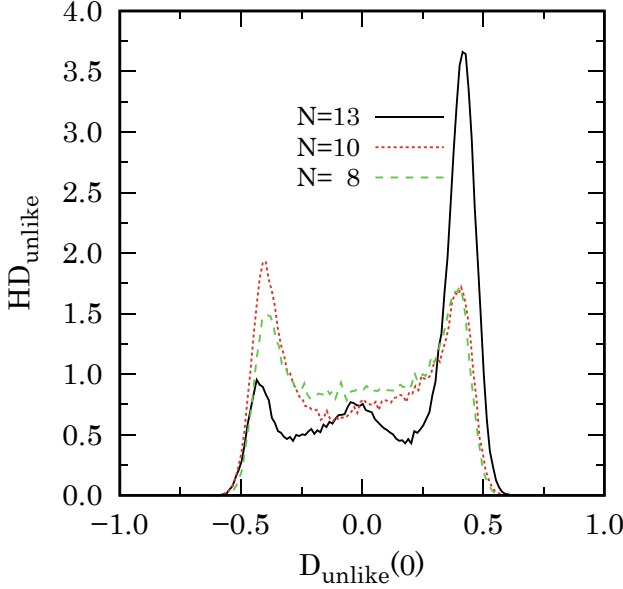


Fig. 8.5 (color online) Histogram of $D_{\text{unlike}}(0)$ block values during the simulation shown in Fig. 8.2. The $N = 13$ data presents a high asymmetry during the evolution of the simulation, which again signals that the simulation was not long enough

for the argument will not violate the detailed balance, required by the Metropolis algorithm, as long as the maximum displacement is chosen $\delta_\theta \geq 2\pi$ so that the probability to go from an angle θ_A to θ_B will be equal to the one to return to θ_A from θ_B always using counterclockwise rotations.

In Fig. 8.6 we show $D_{\text{like}}(z)$ and $D_{\text{unlike}}(z)$ as obtained for $m = 1$, $\bar{g} = 1$, $\bar{\Phi} = 1$, $L = 3$, and four choices of increasing N , in the affine scenario, for the fields $\bar{\phi}_1 = \rho \cos \theta$ and $\bar{\phi}_2 = \rho \sin \theta$. The simulations, an order of magnitude shorter than the one of Fig. 8.2, rapidly converged and we had vanishing $\langle \bar{\phi}_i \rangle$ as required. From the figure we can see how the symmetry $z \rightarrow L - z$ appears to be broken in both two-point functions. In particular the unlike one appears to be oscillating close to the value of zero. This can be seen as an artifact due to the chosen asymmetric expression for the kinetic part of the primitive approximation. The two-point functions, that are now well converged, seem to have a well defined continuum limit $N \rightarrow \infty$. In fact the difference between $D_{\text{like}}(|z| = L/2)$ from $N = 10$ and $N = 8$ is 0.043 but the one from $N = 15$ and $N = 13$ is 0.036. This supports the conclusion that affine quantization leads to a well defined field theory. This is also supported by looking at the renormalized mass and coupling constant [6]: $m_R = 0.101748(8)$, $\bar{g}_R = 1.50000(1)$ for $N = 8$, $m_R = 0.097307(8)$, $\bar{g}_R = 1.50000(2)$ for $N = 10$, $m_R = 0.08949(4)$, $\bar{g}_R = 1.50000(3)$ for $N = 13$, $m_R = 0.08398(6)$, $\bar{g}_R = 1.49997(4)$ for $N = 15$. We can see how the renormalized coupling constant remains constant upon the increase of N .

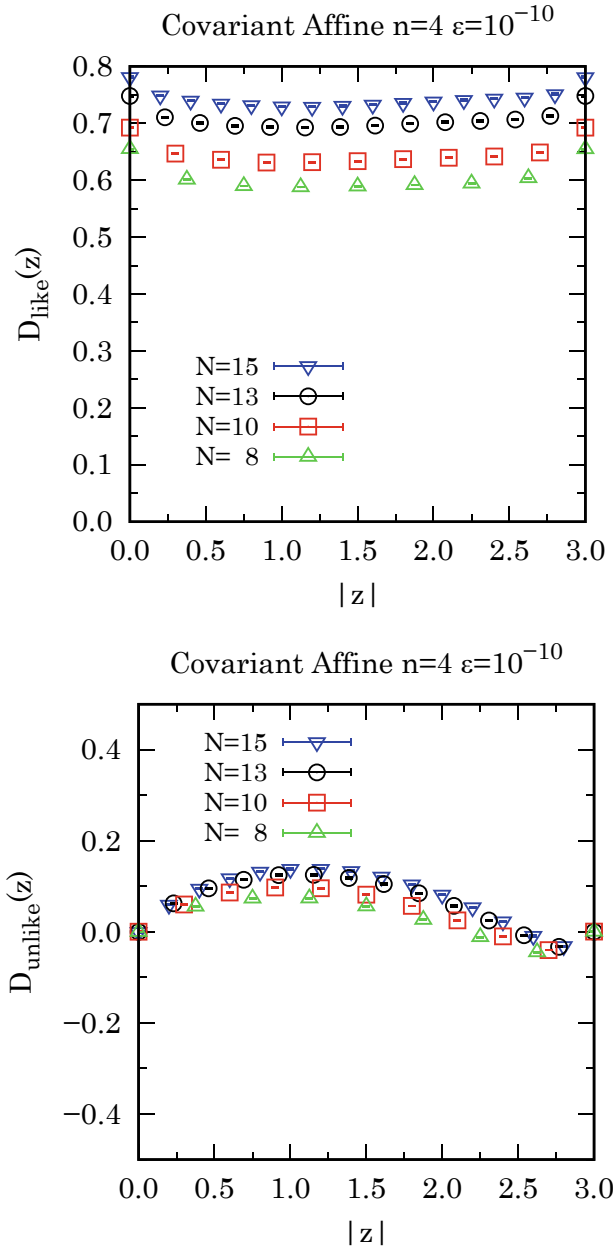


Fig. 8.6 (color online) Two-point functions, $D_{\text{like}}(z)$ (top panel) and $D_{\text{unlike}}(z)$ (bottom panel), of Eq. (8.16) for the complex scalar Higgs field $\tilde{\varphi} = \phi_1 + i\phi_2 = \rho \exp(i\theta)$ subject to affine quantization with a self-interaction potential density of the form $V = \frac{1}{2}m^2\rho^2 + g(\rho^2 - \Phi^2)^2$ in Eq. (8.3) with $m = 1, \bar{g} = 1, \bar{\Phi} = 1, L = 3$ in Eq. (8.21) and increasing $N = 8, 10, 13, 15$. The simulation used $M = 10^6$ MC steps and started from the initial condition $\rho = \epsilon = 10^{-10}$. On the abscissa axis we have $|z| = \sqrt{z_0^2 + z_1^2 + \dots + z_s^2}$ which is a length

Summarizing, here we studied, through Monte Carlo simulations, the two-point function of a classical Euclidean covariant complex scalar field of mass m subject to the Higgs Mexican-hat potential in four spacetime dimensions, treated either with canonical quantization and with affine quantization. And we analyzed the continuum limit at finite fixed volume. The finite volume constraint rules out the formation of the massless Goldstone boson due to the spontaneous symmetry breaking of the continuous phase symmetry $\varphi(x) \rightarrow e^{i\theta(x)}\varphi(x)$ that we continue to observe in the simulations even if only as a smooth transition (free energies in finite volume systems are always analytic).

We first studied the path integral in the two real fields ϕ_1 and ϕ_2 with $\varphi = \phi_1 + i\phi_2$ through standard Metropolis [13] simulations. In the canonical case we found rapidly converging simulations: the unlike two-point function is zero everywhere and the like one shows the approach to the continuum through a diverging value at the origin. It is periodic of periodicity L and satisfies the symmetry $z \rightarrow L - z$ as it should. It has a minimum at half simulation box $|z| = L/2$ close to zero, indicating that the scalar field theory is in the unbroken phase under canonical quantization, at the chosen couplings and dimension.

In the affine case, we found that due to the appearance of the forbidden region around the origin $\varphi \approx 0$, the ergodicity of the random walk is broken. Once the field spontaneously breaks the symmetry falling in the circle of vacua, it can only rotate around the peak in the potential at the origin. Therefore very long simulations are necessary in order to find reliable results for the expectation values. More so approaching the continuum. This suggested to change variables from ϕ_1 and ϕ_2 to the modulus ρ and the argument θ of the complex field, with $\varphi = \rho \exp(i\theta)$ and choose an asymmetric transition rule for the argument move in the Metropolis algorithm in order to allow only for counterclockwise rotations around the origin. This proved an effective way to overcome the ergodicity problem encountered previously, and the simulations converged quickly.

The approach to the continuum appears to be well behaved also for the affine case where the unlike two-point function continues to be everywhere close to zero and the like one develops a minimum at half simulation box higher than the one observed in the canonical case indicating that the system under affine quantization is in the broken phase. Therefore, we can say that affine quantization produces a meaningful quantum field theory. It would be interesting to carry on a detailed and systematic study of the approach to the continuum of the renormalized coupling constant in order to understand whether the affine approach is able to produce a non-trivial [7–10, 16] interacting field theory in the continuum limit also for the present case of a complex scalar field subject to the Higgs potential, as was done in our previous works for scalar real fields [5, 6]. This would solve the problem of the believed triviality of the canonical Higgs particle in four spacetime dimensions.

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Chapter 9

Conclusions



l'amor che move il sole e l'altre stelle.

*Dante Alighieri
La Divina Commedia (canto XXXIII paradiso)*

Abstract In this chapter, we give our concluding remarks pointing out the importance of our study for Quantum Gravity.

It is then time to conclude this short book. And I would like to begin quoting John's own words on our beautiful joint work [1] which I just helped in editing and submitting to a proper journal:

Could it be the time now to pass from CQ to AQ to solve difficult problems? Perhaps new procedures can help. The passing of years can often lead to the introduction of improved procedures. For example, very early, people on horses took around the mail, then trains, then cars, switching to the internet, etc. Likewise, first there was CQ, now AQ, which is added to become CQ & AQ = EQ, known as 'Enhanced Quantization' [2]. It has introduced a huge jump that greatly extends quantization procedures, along with a noteworthy proof that, essentially, $AQ \rightarrow CQ$.

In an artistic sense, CQ represents the beautiful surface of a brick made of pure gold, while AQ represents the wonderful interior of the same gold brick. Hence, moving around within an inside path, AQ points can reach a point on the CQ surface!

While the half-harmonic oscillator using AQ was shown to be valid [3], the validity of AQ for field theories or for gravity are not as yet proved to be true, and there are opportunities for others to test their out coming. While every attempt to maintain correctness has been the rule, something may still have been overlooked. The goal of improvement of every step is open to consideration and further recommendation.

As for myself I think that the beauty of a geometric prescription of quantization puts on the same ground CQ, where the Hilbert space has a constant positive curvature, and AQ, where the Hilbert space has a constant negative curvature. I really hope that AQ will in the future appear in graduate students university textbooks or even undergraduates ones. Maybe this brief book can become a small step forward in the process toward that goal!

John, for example, thinks [4] that already the simple square well problem is treated wrongly on current quantum mechanics students books. In fact, Schrödinger's equation $\hat{H}\Psi(q) = E\Psi(q)$ is violated already for the ground state which is given by a cosine within the infinite well and zero outside of it. So that on the left-hand side of Schrödinger's equation the kinetic energy term, $-\frac{\hbar^2}{2m}\Psi''(q)$, with its second-order derivative, produces evidently a delta function which is not balanced on the right-end side of the equation! The same problem occurs in the half-harmonic oscillator [3]. AQ should serve as an extension of CQ in the sense that where CQ exists AQ is useless and vice versa AQ can describe systems for which CQ fails. Moreover, AQ reduces to CQ in the proper limit. For example, AQ for the harmonic oscillator on a half-line $q > b$ reduces to CQ for the harmonic oscillator on the full line in the limit $b \rightarrow -\infty$ as is proved in Ref. [5].

AQ has the very important property that it can only exist if there are *missing parts of space*, and that is shown by incomplete regions that still remain, e.g., $q > 0$, $|q| > 0$, $q^2 < b^2$, $q^2 > b^2$, etc., in quantum mechanics or $\varphi(x) > 0$, $|\varphi(x)| > 0$, $\varphi(x)^2 < b^2$, $\varphi(x)^2 > b^2$, etc., in field theory [5]. This new quantization procedure has proven itself very well in dealing with examples that only have an *incomplete space*. It is that fact which AQ overcomes by introducing a vast variety of parts of incomplete space, such as the mentioned retained space. Only AQ can correctly solve all examples that have missing space regions, and it can do it correctly only with remaining space examples. AQ knows where space ends and can treat "quantum walls", a gift from Nature! This can be used for a proper description of quantum black holes.

In our journey through the book, we saw how AQ is probably the best candidate we have to solve the triviality issue that plagues many self-interacting Euclidean relativistic quantum scalar field theories in n spacetime dimensions like the $(\varphi^r)_n$, that have a self interaction of the form $|\varphi|^r$, covariant ones for $r \geq 2n/(n-2)$ or the ultralocal ones for $r > 2$ and any n . It accomplishes this task just by introducing in the Hamiltonian density a self-interaction *effective* term $\propto \hbar^2/\varphi^2$ which removes any region where $\varphi = 0$ since that term would diverge there. The most important change is that $\varphi \neq 0$ and now that equation has been fully removed. Observe, that CQ requires $0 \leq |\varphi(x)| < \infty$, while AQ seeks to find missing equations which shows that a *specific field value, namely, $\varphi(x) = 0$ is removed, or explained differently, now $0 < |\varphi(x)| < \infty$* . This has been carefully studied and confirmed numerically with the path integral Monte Carlo method both for real and for complex (only for the covariant case) scalar fields.

All this will be of much help in the validation of the Higgs sector of the Standard Model [6] and the quest for a proper quantization of Einstein's general relativity field equations¹ [1]. AQ may solve all problems!

Professor Klauder has featured AQ for gravity for some time, and several recent articles have carried stories regarding gravity [7–10]. Many quantizations about gravity, developed by other authors using CQ or some related procedure, have obtained results, but the validity of these results may be questioned.

The gravity metric, $g_{ab}(x)$, has been re-expressed by the equation $g_{ab}(x) = E_a^i(x)\delta_{ij}E_b^j(x)$, e.g., [11], and has been quantized assuming that $E_a^i(x)$ is like every other set of conventional coordinates that have adopted CQ, and applied them to gravity. However, if just the single point where every $E_a^i(x) = 0$, and $g_{ab}(x) = 0$, it would violate the physics of gravity. This behavior is just like any other multidimensional space that loses just one point, and finds that it should use AQ and not CQ, has been illustrated by [1]. Now imagine that the six variables in the metric have arbitrary values that run over the whole real line, in order to accept only the positive values requires a surface on which the determinant is zero. This remark is addressed to $g(x) = \det[g_{ab}(x)] \neq 0$, and accepts only the part where $g(x) > 0$. This also points toward AQ rather than CQ. The essence of the AQ approach is fairly clear. The classical variables are the momentum $\pi^{ab}(x)$ and the metric $g_{cd}(x)$, along with the determinant of the metric, $g(x) = \det[g_{ab}(x)]$. This leads us to the classical gravity Hamiltonian [12]. Since the dilation variable is actually useful, we choose to offer the Hamiltonian using affine variables. The dilation variable for gravity is the momentric, which gets its name from *momentum* and *metric*, and is $\pi_b^a(x) = \pi^{ac}(x)g_{bc}(x)$. The classical Hamiltonian is given by

$$H = \int \left\{ g(x)^{-1/2} \left[\pi_b^a(x) \pi_a^b(x) - \frac{1}{2} \pi_a^a(x) \pi_b^b(x) \right] + g(x)^{1/2} R(x) \right\} d^3x, \quad (9.1)$$

where $R(x)$ is the three-dimensional Ricci scalar. Using Schrödinger's representation, the quantum dilation operator is $\hat{\pi}_b^a(x) = [\hat{\pi}^{ac}(x)g_{bc}(x) + g_{bc}(x)\hat{\pi}^{ac}(x)]/2$, and the quantum Hamiltonian operator is now given by

$$\mathcal{H} = \int \left\{ \left[\hat{\pi}_b^a(x) g(x)^{-1/2} \hat{\pi}_a^b(x) - \frac{1}{2} \hat{\pi}_a^a(x) g(x)^{-1/2} \hat{\pi}_b^b(x) \right] + g(x)^{1/2} R(x) \right\} d^3x. \quad (9.2)$$

¹ In order to quantize gravity, it is important to render a valid quantization of the Arnowitt, Deser, and Misner classical Hamiltonian. We first choose our new classical variables which include what we also call the dilation field $\pi_b^a(x) = \pi^{ac}(x)g_{bc}(x)$ (summed on c ; here, we denote with Latin indexes only the three spatial components) along with the metric field $g_{ab}(x)$. We don't need to impose any restriction on the metric field because physics already requires that $ds(x)^2 = g_{ab}(x) dx^a dx^b > 0$. The metric can also be diagonalized by non-physical, orthogonal matrices, and then it includes only $g_{11}(x)$, $g_{22}(x)$, & $g_{33}(x)$, each of which must be strictly positive as required by physics (compare the three diagonalized positive metric variables with $q > 0$, which then requires an AQ for the half-harmonic oscillator, and also then appreciate the need for such a quantization that leads to positive results).

This quantum Hamiltonian is ready to help formulate a complete quantum gravity. The extra tasks that quantum gravity requires include applying constraints and tiding up some lesser issues. This is not the place to go further, but proposals for some of these tasks may be found in the papers involving gravity already mentioned, i.e., [7–10].

Naturally, the effective self-interaction term added by AQ renders the quantum mechanics or field theory problems hard to solve analytically but this should not be viewed as a shortcoming since Nature is not necessarily simple and its richness deserves to be fully taken care. Only few toy problems can be solved exactly analytically and when that is not possible for more realistic problems one often has to resort to numerical analysis.

Of course, it is necessary to compare the numerical results from AQ with the laboratory experimental observations and measures. If CQ quantum mechanics and/or quantum field theory is known as one of the most successful theory in contemporary physics, nonetheless it still presents some puzzling inconsistencies and gaps as we have outlined in this book. It would be desirable, in the near future, to compare AQ theoretical analytical and/or numerical predictions with experimental measurements. For example in order to prove the utility of the AQ result for the half-harmonic oscillator we could use a tiny oscillator (like a micromembrane or nanowire) and cool it to cryogenic temperatures.² Or maybe, since the zero point energy of the half-harmonic oscillator treated through AQ is four times the one of the full harmonic oscillator treated with CQ this could be measured in an experiment on the Casimir effect. These experimental issues may be the subject of a next book.³

² Harmonic oscillators have energy levels spaced by $\hbar\omega$. The thermal energy in a harmonic oscillator is given by $k_B T$. If $k_B T \gg \hbar\omega$, then many energy levels of the harmonic oscillator will be occupied and the oscillator will behave like a thermal classical oscillator, not so interesting. The challenge then to creating a quantum harmonic oscillator is to get an oscillator cold enough (or high enough oscillation frequency) such that we have $k_B T \ll \hbar\omega$.

³ After all John during his stay at Bell Labs realized very concrete studies. In one of our email exchanges he wrote me (dated 28 December 2023): “Yes, I had an interesting history. And my year of 22 I was able to influence current radars. Normally they have a fixed altitude of a box with a fixed frequency of signal. That meant if the box was long, then you could not decipher multiple Targets, and if it was very small anymore, and the length head could not reach very far away. I invented by saying that the radar should be sent in long manner but the frequency inside should be linearly increased in value. That overcame the distance problem to get something back again as well as having a changing frequency, it came back with information about how many targets are available. Permission to make it public. I was asked to write the article for the bell labs journal, which I did there was a second author who worked on the technical problems of reality, and then two more authors, who did not at all work on that particular topic, but they claimed they wanted to have the Honor to join us. I know in fact, two more co-authors who knew nothing about it at the time have found a way to enter their place on the title. Around 19 I got the notion of Affine Quantization being able to take on canonical Quantization, and which case space can be shortened and that business thanks to Mr. Afrin! I am still convinced that I have her in quite a station is the proper.” and again, the same day one hour later “To add to my story, when I suggested that the Fourier transform of the radar would be very helpful, my American salary jumped from 300–400 per month. My how with the money has become less useful.”

Looking back at the title of this book, we know that the path integral invented by Richard Feynman gives us an instrument to go back and forth between classical physics ($\hbar \rightarrow 0$ limit) and quantum physics ($\hbar \neq 0$) or in Euclidean time between classical statistical physics (β small) and quantum statistical physics (β large). Since Nature, as we know it today, is quantum we can see path integral as a bridge, that you can travel smoothly back and forth, between the quantum Nature and the classical version contained in it. On the other hand, we can see the coherent states invented by John R. Klauder as a tool that allows you to jump the bridge inside-out.⁴ Now we also know that Nature, as we know it today, follows the laws of general relativity of Albert Einstein which contains Newtonian gravity in the weak gravity and $c \rightarrow \infty$ limit. A mathematically well formulated theory of quantum gravity is still missing. This could be described by a path integral and AQ could be the key ingredient to write such an integral [1, 7].

I see Affine Quantization as a deep vertical subject which operates horizontally among different disciplines like Quantum Physics and Statistical Physics, Field Theory and General Relativity. This transversality opens more questions than gives certainties [15–18].⁵ Therefore, scientific thoughts should certainly benefit from it. In this sense, it is rather amusing and maieutic!

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⁴ In one of our many email exchanges, John wrote me (dated 13 January 2024): “For the Coherent States, it was in my PhD thesis with John Archibald Wheeler in Princeton. I developed that without his suggestion, and I did that all believing it would be a good idea. I called the Coherent State at my time the [13, 14]. John Wheeler sent copies of my PhD thesis to four other professors in different universities and one of them at Harvard picked up on it and did not offer in my work but chose to act like he invented it and call that Coherent States. That was Roy Glauber, and he did not choose to suggest that I had the idea first, but he went on and on, pretending he was the original inventor.”

⁵ These last two publications were written by the Author after John’s death and deal with tensorial field theory rather than scalar field theory which is the subject of the present book.

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